

Critical line of an anisotropic Ising antiferromagnet on square and honeycomb lattices

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Using the approach that we developed recently, we find the critical line of an anisotropic Ising antiferromagnet on two-dimensional square and honeycomb lattices. We extend our previous lemma and conjecture to be useful in the antiferromagnetic system. We find two interesting behaviors: (1) An antiferromagnet is not necessarily most inert at the absolute zero. (2) The field-driven antiferromagnetic phase transition is possible in the honeycomb lattice. [S1063-651X(97)12409-6]

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I. INTRODUCTION

One of the longstanding problems in statistical physics is the Ising model in nonzero magnetic field (except at one dimension) [1,2]. We do not have the precise knowledge of its thermodynamic properties. Particular interest has focused on its critical properties. Although no exact solutions exist, some exact results have been established. The most famous among these results is the Yang-Lee circle theorem [3], which states that the roots of the partition function of an Ising ferromagnet in the complex fugacity plane are distributed on a unit circle. In the thermodynamic limit the root distribution approaches the positive real axis and gives the critical point. The Yang-Lee circle theorem asserts that the critical line of an Ising antiferromagnet is located at $h=0$ for $T < T_c$.

The circle theorem was so useful that there were many attempts to extend it. The theorem was extended to the cases of higher-order Ising model [4], Ising models with multiple spin interactions, the quantum Heisenberg model [5], the classical XY and Heisenberg model [6], and some continuous spin systems [7]. Ruelle [8] extended the theorem to noncircular regions. Lee [9] presented a generalized circle theorem to the asymmetric transitions and further to a continuum system.

For a lattice model in the absence of magnetic field, it is convenient to consider the zeros of the canonical partition function in the complex temperature plane. Fisher [10] proved that for the square lattice Ising model, in the thermodynamic limit, the zeros are distributed on circles and the logarithmic singularity occurs as a consequence of the zero distribution. However, for other lattice Ising models, the zero distributions are complicated [11,12]. The zero distributions of Potts models were studied in [13].

However, for an Ising antiferromagnet in a nonzero magnetic field, no such theorem exists, and the situation is much more complicated. The traditional mean-field methods cannot give reasonable results. The series expansion method was widely used to study the properties of the Ising model in a nonzero field [14]. Müller-Hartmann and Zittartz [15] obtained a good approximation of the critical line of an Ising antiferromagnet on a square lattice by considering an interface free energy. Later Lin and Wu [16] extended this method to the anisotropic Ising antiferromagnet on a triangular lattice. Wu and co-workers [17,18] introduced an ap-

proach mapping the Ising model into the vertex model and considered the critical lines as the invariant of some transformation.

Recently we introduced a new approach considering zeros of the Ising partition function on an elementary cycle of square, triangular and honeycomb lattices, and determined the critical line of an isotropic Ising antiferromagnet on square and honeycomb lattices [19]. In this paper we extend this approach to obtain the critical lines of an anisotropic Ising antiferromagnet on square and honeycomb lattices. We compare our results with those obtained by Müller-Hartmann and Zittartz [15] for an anisotropic antiferromagnet on a square lattice. We confirm that the limiting behavior of the critical line in the low- T limit agrees reasonably with the existing results found by others [15,17,20] with slight differences. We find two interesting behaviors. In the cases of a square lattice with $(K_1 > 0, K_2 < 0)$ and a honeycomb lattice with $(K_1 < 0, K_2 < 0, K_3 < 0)$ and $(K_1 < 0, K_2 > 0, K_3 > 0)$, the critical line has a maximum at a temperature $T_m \neq 0$, which means that for a given magnetic field two phase transitions are possible as predicted by Ziman [21] and confirmed by a Monte Carlo simulation of an Ising antiferromagnet on a body-centered cubic lattice [22]. It also means that the antiferromagnet is not necessarily most inert against demagnetizing field at the absolute zero. In the case of a honeycomb lattice with $(K_1 > 0, K_2 < 0, K_3 < 0)$ a field-driven antiferromagnetic phase transition is possible as predicted in an antiferromagnet on a triangular lattice [16,23].

The paper is organized as follows. In Sec. II we explain our basic approach used in Ref. [19], and extend the lemma conjecture. In Sec. III we consider the square lattice. We present the critical lines, critical temperatures, and T_m . We derive the low- T limit of the critical line, and give a heuristic explanation for the zero temperature critical field. In Sec. IV we repeat the procedure for the honeycomb lattice.

II. BASIC APPROACH

The partition function of an Ising model in magnetic field is given by

$$Z = \sum_{\{s_i\}} \exp \left[\beta \left(\sum_{\langle ij \rangle} K_{ij} s_i s_j + h \sum_i s_i \right) \right], \quad (1)$$

where $s_i = \pm 1$ and K_{ij} is the interaction strength. We con-

sider the simplest case that the sum $\langle ij \rangle$ runs over the pairs of nearest neighbors on the lattices. $K_{ij} > 0$ corresponds to the ferromagnetic case, and $K_{ij} < 0$ to the antiferromagnetic case. The Ising partition function on each elementary cycle of the triangular, square, and honeycomb lattices are

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

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

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

where K_j are the interaction strengths.

Our approach was inspired by the following observation.

Lemma 1: Let the Ising partition function on an elementary cycle of the square, triangular, and honeycomb lattices be $z = z(T, h = 0)$. Make a transformation $\exp(2\beta K_j) \rightarrow i \exp(2\beta |K_j|)$ and thus $z \rightarrow z'$. Then the critical temperatures of an Ising ferromagnet on square, triangular and honeycomb lattices in the absence of magnetic field are given by the real solutions of $z' = 0$.

The transformed partition functions are

$$z'_t = 2i^{3/2}[e^{\beta(K_1+K_2+K_3)} - e^{\beta(-K_1-K_2+K_3)} - e^{\beta(-K_2-K_3+K_1)} - e^{\beta(-K_3-K_1+K_2)}] \\ = 2i^{3/2}(\zeta_1\zeta_2\zeta_3)^{-1/2}(1 - \zeta_1\zeta_2 - \zeta_2\zeta_3 - \zeta_3\zeta_1), \tag{5}$$

$$z'_s = 2[-e^{2\beta(K_1+K_2)} + e^{2\beta(K_1-K_2)} + e^{-2\beta(K_1-K_2)} - e^{-2\beta(K_1+K_2)} + 4] \\ = 2(\zeta_1\zeta_2)^{-1}[(\zeta_1 + \zeta_2)^2 - (1 - \zeta_1\zeta_2)^2], \tag{6}$$

$$z'_h = 2i[-e^{2\beta(K_1+K_2+K_3)} + 4e^{2\beta K_1} + 4e^{2\beta K_2} + 4e^{2\beta K_3} - 4e^{-2\beta K_1} - 4e^{-2\beta K_2} - 4e^{-2\beta K_3} + e^{2\beta(K_1+K_2-K_3)} + e^{2\beta(K_2+K_3-K_1)} + e^{2\beta(K_3+K_1-K_2)} - e^{-2\beta(K_1+K_2-K_3)} - e^{-2\beta(K_2+K_3-K_1)} - e^{-2\beta(K_3+K_1-K_2)} + e^{-2\beta(K_1+K_2+K_3)}] \\ = -2i(\zeta_1\zeta_2\zeta_3)^{-1}[(1 - \zeta_1\zeta_2 - \zeta_2\zeta_3 - \zeta_3\zeta_1)^2 - (\zeta_1 + \zeta_2 + \zeta_3 - \zeta_1\zeta_2\zeta_3)^2]. \tag{7}$$

where $\zeta_j \equiv \exp(-2\beta K_j)$. Indeed, it is easy to verify that the real solutions of $z' = 0$ give the exact zero-field critical temperatures of an Ising ferromagnet: square, $\zeta_1\zeta_2 + \zeta_1 + \zeta_2 = 1$; triangular, $\zeta_1\zeta_2 + \zeta_2\zeta_3 + \zeta_3\zeta_1 = 1$; and honeycomb, $\zeta_1\zeta_2\zeta_3 - \zeta_1\zeta_2 - \zeta_2\zeta_3 - \zeta_3\zeta_1 - \zeta_1 - \zeta_2 - \zeta_3 + 1 = 0$.

The Ising partition function on an elementary cycle of square and honeycomb lattices, Eqs. (3) and (4), are invariant under the symmetry operations, $K_i \rightarrow -K_i$. Equations (6) and (7) have the same symmetry modulo overall sign. For an

Ising antiferromagnet on the square and honeycomb lattices, the zero-field critical conditions [2] were obtained: square, $\zeta_1\zeta_2 + \zeta_1 + \zeta_2 = 1$; and honeycomb, $\zeta_1\zeta_2\zeta_3 - \zeta_1\zeta_2 - \zeta_2\zeta_3 - \zeta_3\zeta_1 - \zeta_1 - \zeta_2 - \zeta_3 + 1 = 0$, where $\zeta_j \equiv \exp(-2\beta |K_j|)$. Thus the critical temperatures of an Ising ferromagnet and an Ising antiferromagnet on the same kind of lattice, square or honeycomb, must be identical in the absence of magnetic field. Accordingly our lemma 1 is extended to:

Lemma 2: Let the Ising partition function on an elementary cycle of the square and honeycomb lattices be $z = z(T, h = 0)$. Make a transformation $\exp(2\beta |K_j|) \rightarrow i \exp(2\beta |K_j|)$, and thus $z \rightarrow z'$. Then the critical temperatures of an Ising antiferromagnet on square and honeycomb lattices in the absence of magnetic field are given by the real solutions of $z' = 0$.

However, our lemma 1 cannot be extended for a triangular lattice due to lack of symmetry.

In 1970 Griffiths [24,25] 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 [25].

We use this postulate and take lemma 2 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 $(\partial h / \partial M)_T = 0$ [26]. For a square lattice Ising model, the spontaneous magnetization is given by [27]

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

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

$$M(T < T_c, h) = g(T, h)[\gamma(T, h)]^{1/8}, \tag{9}$$

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

$$\left(\frac{\partial M}{\partial h} \right)_T = \frac{\partial g}{\partial h} [\gamma(T, h)]^{1/8} + \frac{g}{8} \frac{\partial \gamma}{\partial h} [\gamma(T, h)]^{-7/8}. \tag{10}$$

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 2 to the case of nonzero magnetic field.

Conjecture: Let the Ising partition function on an elementary cycle of square and honeycomb lattices be $z = z(T, h)$. Make a transformation

$$p_j = e^{2\beta |K_j|} \rightarrow p'_j = i e^{2\beta |K_j|} \quad \text{and} \quad |h| \rightarrow f(|h|). \tag{11}$$

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

Let us recall how the conjecture was used to find the critical line of an isotropic Ising antiferromagnet on square and honeycomb lattices [19]. The Ising partition function on an elementary cycle of square and honeycomb lattices, in the isotropic case, can be written as

$$z = \lambda_+^N + \lambda_-^N, \quad (12)$$

where $\lambda_{\pm} = e^{\beta K} [\cosh \beta h \pm (\sinh^2 \beta h + e^{-4\beta K})^{1/2}]$, and N is the number of the edges of an elementary cycle. Making the transformation gives the critical line of an isotropic Ising antiferromagnet on square and honeycomb lattices, which is

$$e^{4\beta|K|} = e^{4\beta_c|K|} \cosh^2 \beta f(|h|) + \sinh^2 \beta f(|h|). \quad (13)$$

To the first-order approximation, $f(h) = 2h/q$, the critical line is given by

$$e^{4\beta|K|} = \cot^2 \left[\frac{\pi(q-2)}{4q} \right] \cosh^2 \left(\frac{2\beta h}{q} \right) + \sinh^2 \left(\frac{2\beta h}{q} \right), \quad (14)$$

where q is the coordination number. Here we used the formula

$$e^{-2\beta_c K} = \tan \left[\frac{\pi(q-2)}{4q} \right]. \quad (15)$$

To the third-order approximation,

$$f(|h|) = A|h| + B|h|^2/|K| + C|h|^3/|K|^2. \quad (16)$$

In our previous work [19] we used a set of coefficients, $A = 0.542\,578$, $B = 0.003\,487\,3$, and $C = -0.003\,532\,95$ for a square lattice to fit the data in Refs. [15,28] and $A = 0.691\,515\,07$, $B = -0.003\,105\,195$, and $C = -0.001\,725\,869$ for a honeycomb lattice to fit the data in Ref. [17].

In the following discussions we will use a popular notation for h and T : $\eta \equiv h/K$ and $\tau \equiv kT/K$. η and τ are dimensionless quantities measuring the magnetic field and temperature.

III. SQUARE LATTICE

The Ising partition function on an elementary cycle of the square lattice in magnetic field is given by

$$z_s(T, h) = e^{2\beta(K_1+K_2)} (e^{4\beta h} + e^{-4\beta h}) + 4(e^{2\beta h} + e^{-2\beta h}) + 2e^{2\beta(K_1-K_2)} + 2e^{-2\beta(K_1-K_2)} + 2e^{-2\beta(K_1+K_2)}. \quad (17)$$

There can be two distinct combinations of coupling coefficients, (K_1, K_2) , for an anisotropic antiferromagnet. We need to work on each case separately.

A. Case (i): $K_1 < 0, K_2 < 0$

The Ising partition function (17) of the square lattice can be rewritten as

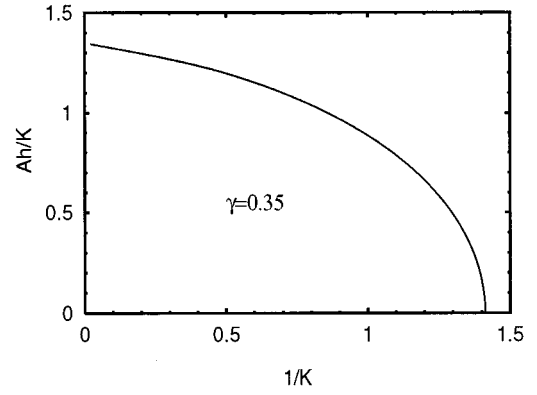


FIG. 1. Critical line of an Ising antiferromagnet on a square lattice: $K_1 < 0$ and $K_2 < 0$.

$$z(T, h) = e^{-2\beta(|K_1|+|K_2|)} (e^{4\beta h} + e^{-4\beta h}) + 4(e^{2\beta h} + e^{-2\beta h}) + 2e^{2\beta(|K_1|-|K_2|)} + 2e^{-2\beta(|K_1|-|K_2|)} + 2e^{2\beta(|K_1|+|K_2|)}. \quad (18)$$

Making the transformation, $\exp(2\beta|K_1|) \rightarrow i \exp(2\beta|K_1|)$, $\exp(2\beta|K_2|) \rightarrow i \exp(2\beta|K_2|)$ and $|h| \rightarrow f(|h|)$, we obtain the critical line as the zero of

$$-e^{-2\beta(|K_1|+|K_2|)} [e^{4\beta f(|h|)} + e^{-4\beta f(|h|)}] + 4[e^{2\beta f(|h|)} + e^{-2\beta f(|h|)}] + 2e^{2\beta(|K_1|-|K_2|)} + 2e^{-2\beta(|K_1|-|K_2|)} - 2e^{2\beta(|K_1|+|K_2|)} = 0. \quad (19)$$

The zero-field limit of Eq. (19) reduces to the Onsager's [29] formula for the critical temperature,

$$1 = \sinh(2\beta|K_1|) \sinh(2\beta|K_2|). \quad (20)$$

We may assume $|K_1| \geq |K_2|$ without loss of generality. Let us define two parameters, $|K_1| = K$ and $|K_2| = \gamma K$. Using the first-order approximation, $f(h) \approx Ah$, we made a sample plot of Eq. (19) in Fig. 1. As the temperature decreases the antiferromagnetic phase of the system tolerates higher and higher demagnetizing field. As K is increased η_c rises monotonically to the maximum value. At the $T \rightarrow 0$ limit, we have

$$Ah_c = |K_1| + |K_2|. \quad (21)$$

The zero field critical temperature, τ_c is an increasing function of γ ; see Fig. 2. Thus as the coupling strength $|K_2|$ increases, the onset of antiferromagnetism occurs at higher and higher temperature.

Let us obtain the approximate form of the critical line in the $T \rightarrow 0$ limit. Since within the first-order approximation $(|K_1| + |K_2|) \approx Ah$ in the $T \rightarrow 0_+$ limit, the largest terms in Eq. (19) are

$$-e^{-2\beta(|K_1|+|K_2|)} e^{4\beta Ah} + 4e^{2\beta Ah} - 2e^{2\beta(|K_1|+|K_2|)} \approx 0. \quad (22)$$

Solving Eq. (22) for $e^{2\beta Ah}$, we obtain

$$e^{2\beta Ah} \approx (2 - \sqrt{2}) e^{2\beta(|K_1|+|K_2|)}, \quad (23)$$

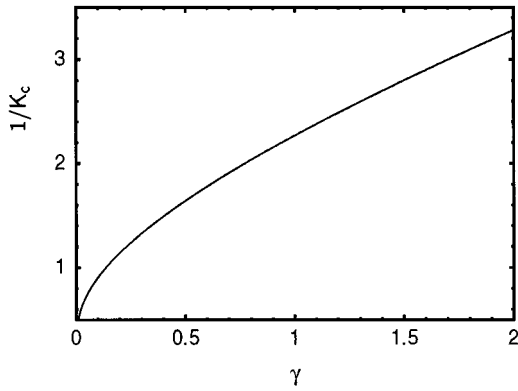


FIG. 2. Critical temperature $\tau_c(\gamma)$ of an Ising antiferromagnet on a square lattice: all cases.

which reduces to

$$Ah \approx -\frac{kT}{2} \ln \frac{2 + \sqrt{2}}{2} + (|K_1| + |K_2|). \quad (24)$$

The constant A is related to the spin configuration of the ground state. The energy is given by $E = |K_1| \sum_{\langle ij \rangle} s_i s_j + |K_2| \sum_{\langle ij \rangle} s_i s_j - h \sum_i s_i$. According to the Gibbs distribution, the energy has the absolute minimum value at the absolute zero temperature. When h is small the minimum energy spin configuration is as shown in Fig. 3(a) and $E = (-|K_1| - |K_2|)N$. Here N is the number of lattice points. This corresponds to an antiferromagnetic state. As h increases enough, the spin configuration changes into a paramagnetic state [Fig. 3(c)] with lower energy $E = (|K_1| + |K_2| - h)N$. The transition takes place when the energies of the two states become identical or $h = 2(|K_1| + |K_2|)$. So we obtain $A = \frac{1}{2}$.

The critical line equation obtained by Müller-Hartmann and Zittartz [15],

$$\cosh \beta h = \sinh(2\beta |K_1|) \sinh(2\beta |K_2|) \quad (25)$$

reduces to $h \approx -kT \ln 2 + 2(|K_1| + |K_2|)$ in the low- T limit.

For a few γ values we computed critical temperatures at a given magnetic field for the two models. They are listed in Table I. Here we used $K(1 + \gamma)/2$ in place of K in using Eq. (16). Although our formula (16) was derived to fit the data given in Refs. [20,25,28] for the isotropic Ising antiferromagnet, the W - K results are in reasonable agreement with the MHZ data to the same extent as in the isotropic case.

B. Case (ii): $K_1 > 0, K_2 < 0$

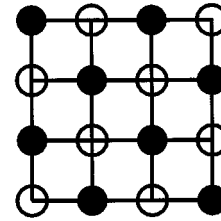
The Ising partition function on an elementary cycle can be rewritten as

$$\begin{aligned} z(T, h) = & e^{2\beta(K_1 - |K_2|)} (e^{4\beta h} + e^{-4\beta h}) + 4(e^{2\beta h} + e^{-2\beta h}) \\ & + 2e^{-2\beta(K_1 + |K_2|)} + 2e^{2\beta(K_1 + |K_2|)} + 2e^{-2\beta(K_1 - |K_2|)}. \end{aligned} \quad (26)$$

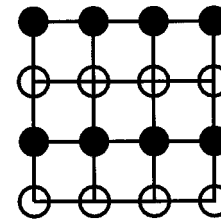
Once again the critical line is given by the zero of the transformed partition function,

$$e^{2\beta(K_1 - |K_2|)} [e^{4\beta f(|h|)} + e^{-4\beta f(|h|)}] + 4[e^{2\beta f(|h|)} + e^{-2\beta f(|h|)}]$$

(a) configuration A



(b) configuration B



(c) configuration C

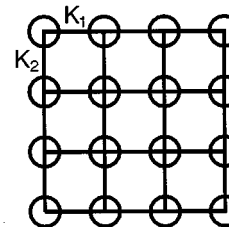


FIG. 3. Possible antiferromagnetic states at $T=0$ on a square lattice.

$$-2e^{-2\beta(K_1 + |K_2|)} - 2e^{2\beta(K_1 + |K_2|)} + 2e^{-2\beta(K_1 - |K_2|)} = 0. \quad (27)$$

Depending on the relative magnitudes of K_1 and $|K_2|$, Eq. (27) behaves differently. Let us again define two parameters, $K_1 = K$ and $|K_2| = \gamma K$. Within the first-order approximation, we made a few plots of Eq. (27) in Fig. 4. As K is increased η_c rises to a maximum value η_m and then decreases to its final value. In the $T \rightarrow 0$ limit, we have

$$Ah_c = |K_2|. \quad (28)$$

Thus it is the negative coupling coefficient that is relevant. The two trends, positive K_1 and negative K_2 , compete and give rise to an interesting behavior. The zero-field critical

TABLE I. Critical temperatures kT/K of an anisotropic Ising antiferromagnet on a square lattice.

| βh | $\gamma=0.75$ | | $\gamma=0.50$ | | $\gamma=0.25$ | |
|-----------|---------------|-----------|---------------|-----------|---------------|-----------|
| | W-K | MHZ | W-K | MHZ | W-K | MHZ |
| 0.1 | 1.968 992 | 1.968 915 | 1.637 868 | 1.637 839 | 1.236 821 | 1.236 873 |
| 0.2 | 1.957 565 | 1.957 287 | 1.637 868 | 1.628 415 | 1.230 119 | 1.230 335 |
| 0.5 | 1.882 829 | 1.881 375 | 1.567 310 | 1.566 882 | 1.186 308 | 1.187 614 |
| 1.0 | 1.674 690 | 1.669 231 | 1.396 968 | 1.394 782 | 1.064 477 | 1.067 701 |
| 2.0 | 1.243 351 | 1.231 334 | 1.044 556 | 1.038 022 | 0.812 737 | 0.815 407 |
| 5.0 | 0.619 114 | 0.613 794 | 0.528 839 | 0.524 837 | 0.432 318 | 0.431 267 |
| 10. | 0.328 576 | 0.327 309 | 0.281 609 | 0.280 532 | 0.234 255 | 0.233 491 |
| 50. | 0.069 083 | 0.069 043 | 0.059 214 | 0.059 180 | 0.049 345 | 0.049 316 |

temperature τ_c is identical to case (i); see Fig. 2. As the temperature decreases the antiferromagnetic phase tolerates higher and higher demagnetizing field. However, the demagnetizing is caused also by the positive K_1 . The maximum η_m is an almost linear function of γ ; see Fig. 5(a). The location of the maximum τ_m rises sharply until $\gamma \approx 0.5$ and then approaches a limiting value, ~ 0.72 ; see Fig. 5(b). Since the zero-field critical temperature τ_c is a linearly increasing function of γ , the relative location of the maximum, τ_m/τ_c shifts to the limit 0 as γ is increased.

Physically τ_m is the temperature at which the antiferromagnet is most inert against the demagnetizing field. We therefore see that τ_m is not necessarily the absolute zero

when the two coupling coefficients have different signs. This also means that for a given magnetic field two phase transitions are possible at two different temperatures, as predicted by Ziman [21] and confirmed by a Monte Carlo simulation of an Ising antiferromagnet on a body-centered-cubic lattice [22].

In order to obtain the approximate form of the critical line in the $T \rightarrow 0$ limit, let us use the first-order approximation for $f(h)$ and find the largest terms in Eq. (27). Since $2|K_2| < Ah$ in the $T \rightarrow 0_+$ limit, the largest terms in Eq. (27) are,

$$e^{2\beta(K_1 - |K_2|)} e^{4\beta Ah} + 4e^{2\beta Ah} - 2e^{2\beta(K_1 + |K_2|)} \approx 0 \quad (29)$$

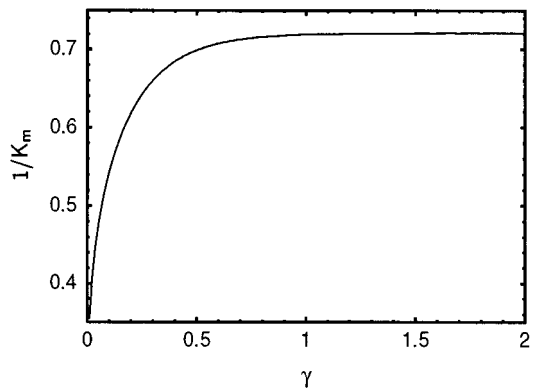
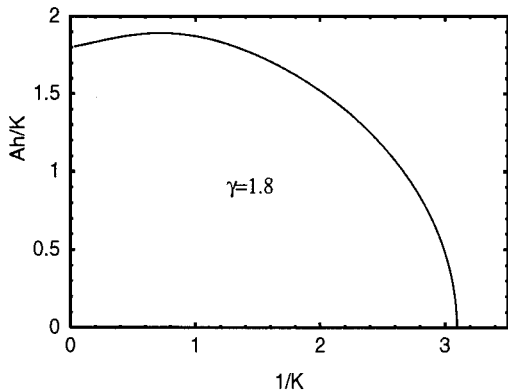
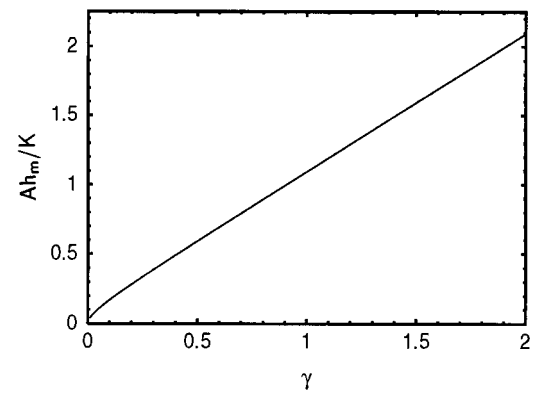
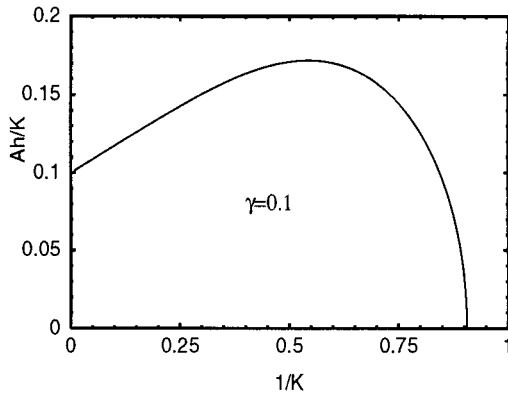


FIG. 4. Critical lines of an Ising antiferromagnet on a square lattice: $K_1 > 0$ and $K_2 < 0$.

FIG. 5. The most inert points: $A\eta_m(\gamma)$ and $\tau_m(\gamma)$: $K_1 > 0$ and $K_2 < 0$.

or

$$e^{2\beta(K_1-|K_2|)}e^{4\beta Ah} - 2e^{2\beta(K_1+|K_2|)} \approx 0, \quad (30)$$

which reduces to

$$Ah \approx \frac{kT}{4} \ln 2 + |K_2|. \quad (31)$$

The positive slope of the critical line at $T=0$ means that $\tau_m \neq 0$.

Let us find the constant A from the spin configuration of the ground state. The energy is given by $E = -K_1 \sum_{\langle ij \rangle} s_i s_j + |K_2| \sum_{\langle ij \rangle} s_i s_j - h \sum_i s_i$. When h is small

the minimum energy spin configuration is shown in Fig. 3(b) (K_1 is the horizontal link) and $E = (-K_1 - |K_2|)N$. This corresponds to an antiferromagnetic state. As h increases, the spin configuration changes into a paramagnetic state [Fig. 3(c)] with lower energy $E = (-K_1 + |K_2| - h)N$. The transition takes place when the energies of the two states become identical or $h = 2|K_2|$. So $A = \frac{1}{2}$ again.

IV. HONEYCOMB LATTICE

The Ising partition function on an elementary cycle of the honeycomb lattice in magnetic field is

$$\begin{aligned} z(T, h) = & e^{2\beta(K_1+K_2+K_3)}(e^{6\beta h} + e^{-6\beta h}) + 2(e^{2\beta K_1} + e^{2\beta K_2} + e^{2\beta K_3})(e^{4\beta h} + e^{-4\beta h}) + [2(e^{2\beta K_1} + e^{2\beta K_2} + e^{2\beta K_3} + e^{-2\beta K_1} \\ & + e^{-2\beta K_2} + e^{-2\beta K_3}) + e^{-2\beta(K_2+K_3-K_1)} + e^{-2\beta(K_3+K_1-K_2)} + e^{-2\beta(K_1+K_2-K_3)}](e^{2\beta h} + e^{-2\beta h}) + 2e^{2\beta(K_2+K_3-K_1)} \\ & + 2e^{2\beta(K_3+K_1-K_2)} + 2e^{2\beta(K_1+K_2-K_3)} + 4e^{-2\beta K_1} + 4e^{-2\beta K_2} + 4e^{-2\beta K_3} + 2e^{-2\beta(K_1+K_2+K_3)}. \end{aligned} \quad (32)$$

There can be three distinct combinations of coupling coefficients, (K_1, K_2, K_3) , for an antiferromagnet. We need to work on each case separately.

A. Case (i): $K_1 < 0, K_2 < 0, K_3 < 0$

Let us rewrite Eq. (32) in terms of magnitudes of coupling coefficients, $|K_i|$:

$$\begin{aligned} z(T, h) = & e^{-2\beta(|K_1|+|K_2|+|K_3|)}(e^{6\beta h} + e^{-6\beta h}) + 2(e^{-2\beta|K_1|} + e^{-2\beta|K_2|} + e^{-2\beta|K_3|})(e^{4\beta h} + e^{-4\beta h}) + [2(e^{-2\beta|K_1|} + e^{-2\beta|K_2|} \\ & + e^{-2\beta|K_3|} + e^{2\beta|K_1|} + e^{2\beta|K_2|} + e^{2\beta|K_3|}) + e^{2\beta(|K_2|+|K_3|-|K_1|)} + e^{2\beta(|K_3|+|K_1|-|K_2|)} + e^{2\beta(|K_1|+|K_2|-|K_3|)}](e^{2\beta h} + e^{-2\beta h}) \\ & + 2e^{-2\beta(|K_2|+|K_3|-|K_1|)} + 2e^{-2\beta(|K_3|+|K_1|-|K_2|)} + 2e^{-2\beta(|K_1|+|K_2|-|K_3|)} + 4e^{2\beta|K_1|} + 4e^{2\beta|K_2|} + 4e^{2\beta|K_3|} \\ & + 2e^{2\beta(|K_1|+|K_2|+|K_3|)}. \end{aligned} \quad (33)$$

Making the transformation we obtain the critical line,

$$\begin{aligned} e^{-2\beta(|K_1|+|K_2|+|K_3|)}[e^{6\beta f(|h|)} + e^{-6\beta f(|h|)}] - 2(e^{-2\beta|K_1|} + e^{-2\beta|K_2|} + e^{-2\beta|K_3|})[e^{4\beta f(|h|)} + e^{-4\beta f(|h|)}] + [2(-e^{-2\beta|K_1|} - e^{-2\beta|K_2|} \\ - e^{-2\beta|K_3|} + e^{2\beta|K_1|} + e^{2\beta|K_2|} + e^{2\beta|K_3|}) + e^{2\beta(|K_2|+|K_3|-|K_1|)} + e^{2\beta(|K_3|+|K_1|-|K_2|)} + e^{2\beta(|K_1|+|K_2|-|K_3|)}][e^{2\beta f(|h|)} + e^{-2\beta f(|h|)}] \\ - 2e^{-2\beta(|K_2|+|K_3|-|K_1|)} - 2e^{-2\beta(|K_3|+|K_1|-|K_2|)} - 2e^{-2\beta(|K_1|+|K_2|-|K_3|)} + 4e^{2\beta|K_1|} + 4e^{2\beta|K_2|} + 4e^{2\beta|K_3|} \\ - 2e^{2\beta(|K_1|+|K_2|+|K_3|)} = 0. \end{aligned} \quad (34)$$

We may assume $|K_1| \geq |K_2| \geq |K_3|$ without loss of generality. Depending on the relative magnitudes of $|K_1|$, $|K_2|$, and $|K_3|$, Eq. (34) behaves differently. Within the first-order approximation, we made a few plots of Eq. (34) for different combinations of (γ_2, γ_3) in Fig. 6. We notice a few facts.

(i) The $T=0$ limit of η_c depends only on the least negative coupling coefficient,

$$Ah_c = 2|K_3|. \quad (35)$$

(ii) If $\gamma_2 = \gamma_3$, η_c monotonically increases to $2\gamma_3$ as K is increased.

(iii) If $\gamma_2 \neq \gamma_3$, η_c reaches a maximum at (η_m, τ_m) and then decreases to its final value as K is increased.

We made a contour plot of $(\gamma_2, \gamma_3, \tau_c)$ in Fig. 7. For a given value of γ_3 , τ_c is a monotonically increasing function of γ_2 , and vice versa. As a matter of fact, along any direction

in the γ_2 - γ_3 plane its profile looks like Fig. 2. The contours of $(\gamma_2, \gamma_3, A\eta_m)$ are shown in Fig. 8(a). Along any direction in the γ_2 - γ_3 plane its profile looks like Fig. 5(a) and it is steepest along the direction $\gamma_2 = \gamma_3$. We show the contours of $(\gamma_2, \gamma_3, \tau_m)$ in Fig. 8(b). Along the direction $\gamma_2 = \gamma_3$ it does not change at all, but as you go away from this direction its slope becomes steeper and its profile is a convex curve as in Fig. 2.

In order to obtain the approximate form of the critical line in the $T \rightarrow 0$ limit, let us find the largest terms in Eq. (34) to the first-order approximation of $f(h)$. Since $Ah \approx 2|K_3|$ in the $T \rightarrow 0_+$ limit and $|K_3|$ is smaller than $|K_1|$ and $|K_2|$, we obtain

$$\begin{aligned} e^{-2\beta(|K_1|+|K_2|+|K_3|)}e^{6\beta Ah} - 2e^{-2\beta|K_3|}e^{4\beta Ah} \\ + e^{2\beta(|K_1|+|K_2|-|K_3|)}e^{2\beta Ah} - 2e^{2\beta(|K_1|+|K_2|+|K_3|)} \approx 0. \end{aligned} \quad (36)$$

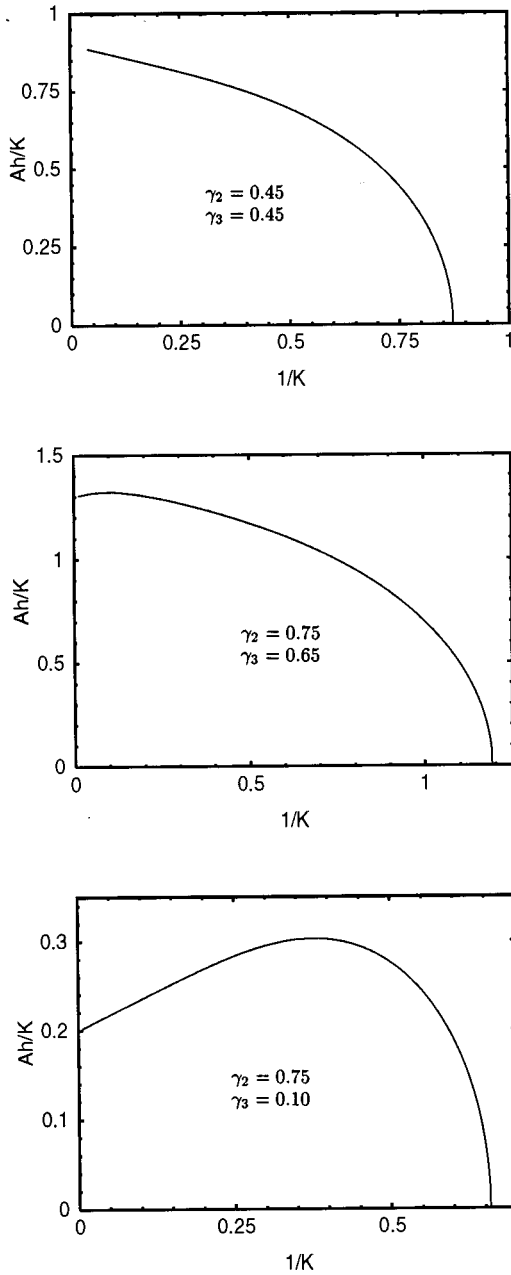


FIG. 6. Critical lines of an Ising antiferromagnet on a honeycomb lattice: $K_1 < 0$, $K_2 < 0$, and $K_3 < 0$.

or, upon discarding smaller terms,

$$e^{2\beta(|K_1|+|K_2|-|K_3|)}e^{2\beta Ah} - 2e^{2\beta(|K_1|+|K_2|+|K_3|)} \approx 0, \quad (37)$$

which reduces to

$$Ah \approx \frac{1}{2}kT \ln 2 + 2|K_3|. \quad (38)$$

The slope of the critical line at $T=0$ is positive, which implies that the most inert temperature is not zero, $\tau_m \neq 0$. The $T \rightarrow 0$ limit of Ah depends only on the least negative coupling coefficient, K_3 .

In the exceptional case when $K_2 = K_3$, instead of Eq. (36), we have

$$e^{-2\beta(|K_1|+2|K_3|)}e^{6\beta Ah} - 4e^{-2\beta|K_3|}e^{4\beta Ah} + 4e^{2\beta|K_1|}e^{2\beta Ah}$$

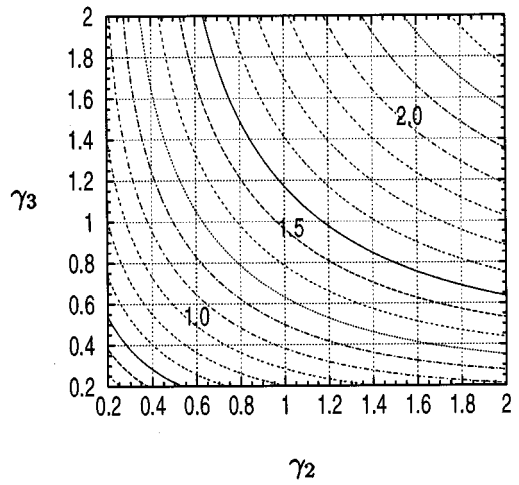


FIG. 7. Critical temperature $\tau_c(\gamma_2, \gamma_3)$ of an Ising antiferromagnet on a honeycomb lattice: all cases.

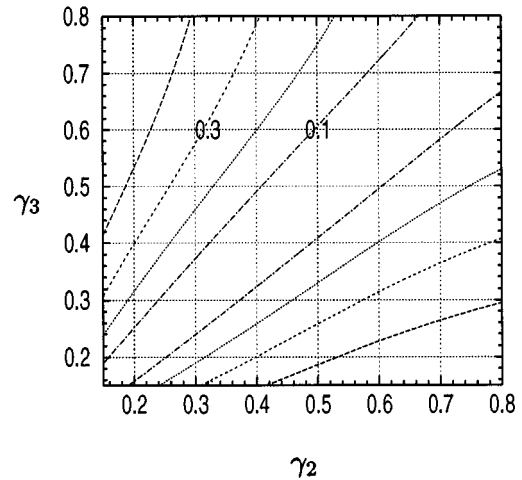
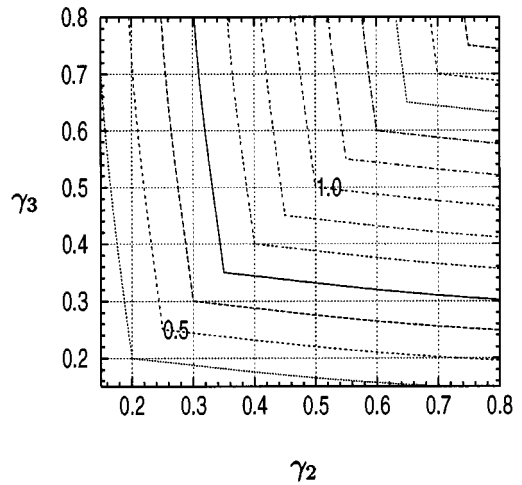


FIG. 8. The most inert points: $A\eta_m(\gamma_2, \gamma_3)$ and $\tau_m(\gamma_2, \gamma_3)$: $K_1 < 0$, $K_2 < 0$, and $K_3 < 0$.

$$-2e^{2\beta(|K_1|+2|K_3|)} \approx 0. \quad (39)$$

In the $T \rightarrow 0$ limit, only the last two terms of Eq. (39) are dominant and thus we have,

$$Ah \approx -\frac{1}{2}kT \ln 2 + 2|K_3|. \quad (40)$$

The slope of the critical line at $T=0$ is negative in this case.

In order to determine the constant A let us again consider the spin configuration of the ground state. The energy is $E = |K_1| \sum_{\langle ij \rangle} s_i s_j + |K_2| \sum_{\langle ij \rangle} s_i s_j + |K_3| \sum_{\langle ij \rangle} s_i s_j - h \sum_i s_i$. When h is small, the lowest energy spin configuration is as shown in Fig. 9(a), and $E = (-|K_1| - |K_2| - |K_3|)N/2$. This corresponds to an antiferromagnetic state. If h increases enough, it settles in a paramagnetic state [Fig. 9(d)] with a lower energy $E = (|K_1| + |K_2| + |K_3| - 2h)N/2$. The transition takes place when the energies of the two states become identical and $h = |K_1| + |K_2| + |K_3|$. Thus we obtain $A = 2|K_3| / (|K_1| + |K_2| + |K_3|) = 2\gamma_3 / (1 + \gamma_2 + \gamma_3)$. A depends on the ratio of the coupling constants. This yields $A = \frac{2}{3}$ in the isotropic case.

B. Case (ii): $K_1 < 0, K_2 > 0, K_3 > 0$

Rewriting Eq. (32) in terms of magnitudes of coupling coefficients, we obtain the Ising partition function on an elementary cycle,

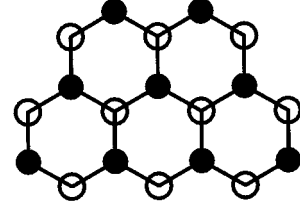
$$\begin{aligned} z(T, h) = & e^{2\beta(K_2+K_3-|K_1|)}(e^{6\beta h} + e^{-6\beta h}) + 2(e^{-2\beta|K_1|} + e^{2\beta K_2} \\ & + e^{2\beta K_3})(e^{4\beta h} + e^{-4\beta h}) + [2(e^{2\beta|K_1|} + e^{2\beta K_2} \\ & + e^{2\beta K_3} + e^{-2\beta|K_1|} + e^{-2\beta K_2} + e^{-2\beta K_3}) \\ & + e^{-2\beta(|K_1|+K_2+K_3)} + e^{-2\beta(-|K_1|+K_2-K_3)} \\ & + e^{-2\beta(-|K_1|+K_3-K_2)}](e^{2\beta h} + e^{-2\beta h}) \\ & + 2e^{2\beta(|K_1|+K_2+K_3)} + 2e^{2\beta(-|K_1|+K_2-K_3)} \\ & + 2e^{2\beta(-|K_1|+K_3-K_2)} + 4e^{2\beta|K_1|} + 4e^{-2\beta K_2} \\ & + 4e^{-2\beta K_3} + 2e^{-2\beta(-|K_1|+K_2+K_3)}. \end{aligned} \quad (41)$$

Making the transformation we obtain the equation for the critical line,

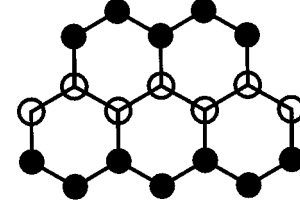
$$\begin{aligned} e^{2\beta(K_2+K_3-|K_1|)}(e^{6\beta f(|h|)} + e^{-6\beta f(|h|)}) + 2(-e^{-2\beta|K_1|} + e^{2\beta K_2} \\ + e^{2\beta K_3})(e^{4\beta f(|h|)} + e^{-4\beta f(|h|)}) + [2(e^{2\beta|K_1|} + e^{2\beta K_2} \\ + e^{2\beta K_3} - e^{-2\beta|K_1|} - e^{-2\beta K_2} - e^{-2\beta K_3}) \\ + e^{-2\beta(|K_1|+K_2+K_3)} + e^{-2\beta(-|K_1|+K_2-K_3)} \\ + e^{-2\beta(-|K_1|+K_3-K_2)}](e^{2\beta f(|h|)} + e^{-2\beta f(|h|)}) \\ - 2e^{2\beta(|K_1|+K_2+K_3)} - 2e^{2\beta(-|K_1|+K_2-K_3)} \\ - 2e^{2\beta(-|K_1|+K_3-K_2)} + 4e^{2\beta|K_1|} - 4e^{-2\beta K_2} - 4e^{-2\beta K_3} \\ - 2e^{-2\beta(-|K_1|+K_2+K_3)} = 0. \end{aligned} \quad (42)$$

We may assume $K_2 \geq K_3$ without loss of generality. Depending on the relative magnitudes of $|K_1|$, K_2 , and K_3 , the

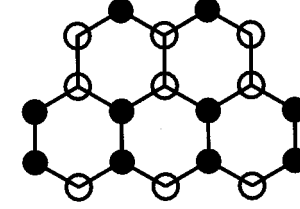
(a) configuration A



(b) configuration B



(c) configuration C



(d) configuration D

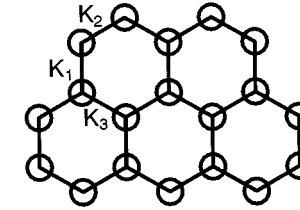


FIG. 9. Possible antiferromagnetic states at $T=0$ on a honeycomb lattice.

behaviors of Eq. (42) are quite different. Let us define three parameters, $|K_1| = K$, $K_2 = \gamma_2 K$, and $K_3 = \gamma_3 K$. We made a few plots of Eq. (42) for different combinations of (γ_2, γ_3) in Fig. 10. We notice a few facts.

(i) The $T=0$ limit of h_c is, for all combinations of (γ_2, γ_3) ,

$$Ah_c = \min\left(\frac{2}{3}|K_1|, 2K_3\right). \quad (43)$$

(ii) Case $\gamma_2 = \gamma_3$: as K is increased, if $\gamma_3 \leq \frac{1}{3}$, $A \eta_c$ monotonically increases to $2\gamma_3$, implying that $Ah_c \rightarrow 2K_3$. Otherwise, η_c reaches a maximum and then decreases to its final

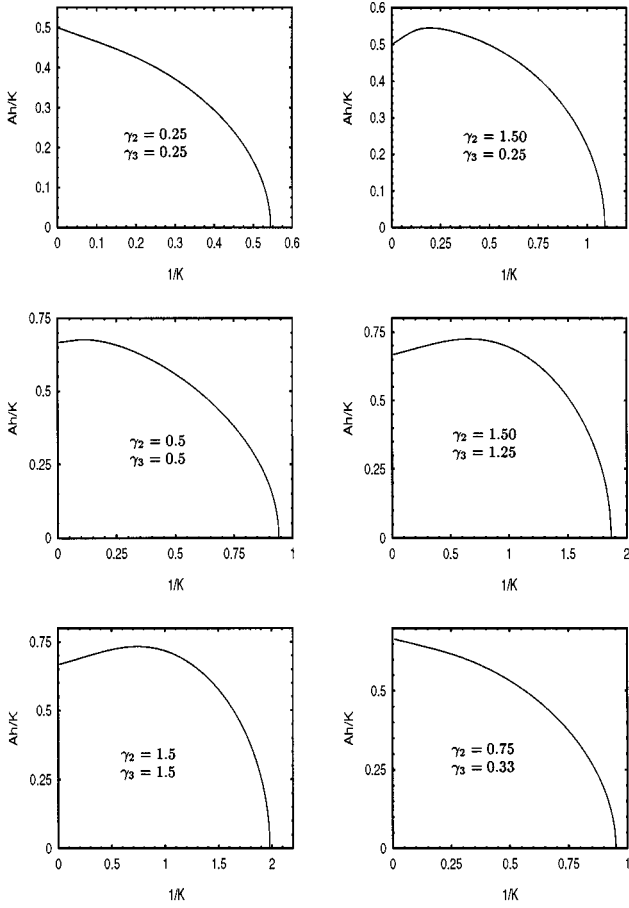


FIG. 10. Critical lines of an Ising antiferromagnet on a honeycomb lattice: $K_1 < 0$, $K_2 > 0$, and $K_3 > 0$.

value, $\frac{2}{3}$, implying that $Ah_c \rightarrow \frac{2}{3}|K_1|$. The maximum value of η_c is an increasing function of γ_3 .

(iii) Case $\gamma_2 \neq \gamma_3$: as K is increased, at $\gamma_2 = \frac{1}{3}$ or $\gamma_3 = \frac{1}{3}$ (implying $2K_3 = \frac{2}{3}|K_1|$), $A\eta_c$ monotonically increases to $\frac{2}{3}|K_1|$. Otherwise η_c reaches a maximum and then decreases to its final value as K is increased. The maximum value of η_c is an increasing function of γ_3 .

We made a contour plot of $(\gamma_2, \gamma_3, \tau_c)$, which is identical to Fig. 7. The contours of $(\gamma_2, \gamma_3, A\eta_m)$ are shown in Fig. 11(a). We need to consider only the upper region of the diagonal $\gamma_2 = \gamma_3$ where the condition $\gamma_2 \geq \gamma_3$ is satisfied. Its profile is no longer a straight line but a convex curve like that of Fig. 2. In the region $\gamma_3 \leq \frac{1}{3}$ the contour rises sharply across the line $\gamma_3 = \text{const}$, but hardly changes along the line. Beyond the line $\gamma_3 = \frac{1}{3}$ it gradually rises. Along the direction $\gamma_2 = \text{const}$ it is steeper than along the diagonal line. The contours of $(\gamma_2, \gamma_3, \tau_m)$ are shown in Fig. 11(b). There are valleys along $\gamma_3 = \frac{1}{3}$ and $\gamma_2 = \gamma_3 \leq \frac{1}{3}$, where the maximum occurs only at $\tau_m = 0$. As you go away from these two lines the location of the maximum shifts towards the zero-field critical temperature.

In order to obtain the approximate form of the critical line in the $T \rightarrow 0$ limit, let us find the largest terms in Eq. (42) within the first-order approximation. Let us consider the case, $\gamma_2 \neq \gamma_3$ first:

$$e^{2\beta(K_2 + K_3 - |K_1|)} e^{6\beta Ah} + 2e^{2\beta K_2} e^{4\beta Ah} + e^{2\beta(|K_1| + K_2 - K_3)} e^{2\beta Ah}$$

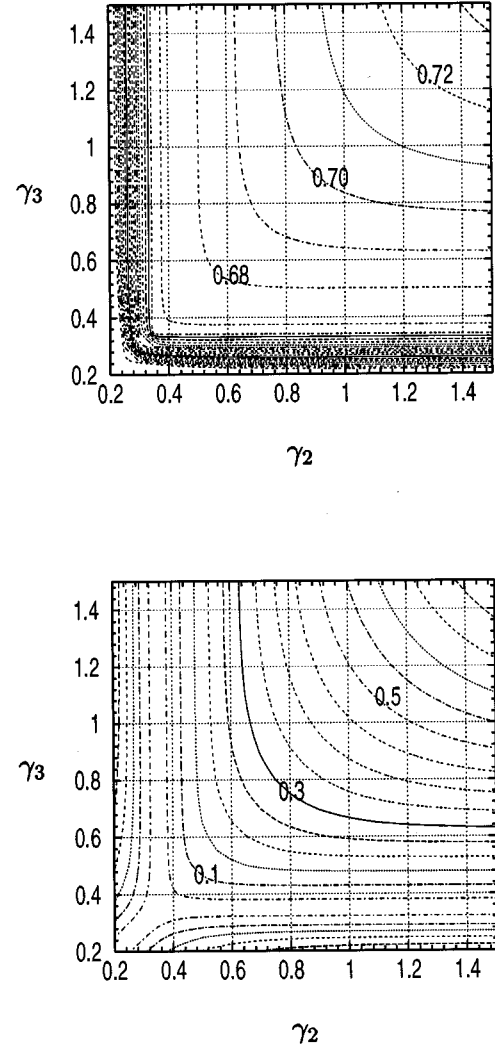


FIG. 11. The most inert points: $A\eta_m(\gamma_2, \gamma_3)$ and $\tau_m(\gamma_2, \gamma_3)$: $K_1 < 0$, $K_2 > 0$, and $K_3 > 0$.

$$-2e^{2\beta(|K_1| + K_2 + K_3)} \approx 0, \quad (44)$$

There are two cases that we have to consider: (a) $\gamma_3 < \frac{1}{3}$ and (b) $\gamma_3 > \frac{1}{3}$.

Case (ii-a): $\gamma_3 < \frac{1}{3}$

Since $Ah \approx 2K_3$ in the $T \rightarrow 0_+$ limit, the two largest terms in Eq. (44) are,

$$e^{2\beta(|K_1| + K_2 - K_3)} e^{2\beta Ah} - 2e^{2\beta(|K_1| + K_2 + K_3)} \approx 0, \quad (45)$$

which reduces to

$$Ah \approx \frac{1}{2} kT \ln 2 + 2K_3. \quad (46)$$

Again the slope of the critical line at $T=0$ is positive. The $T \rightarrow 0$ limit of Ah depends only on the smaller of the two positive coupling coefficient, K_3 .

Case (ii-b): $\gamma_3 > \frac{1}{3}$

Since $Ah \approx \frac{2}{3}|K_1|$ in the $T \rightarrow 0_+$ limit, the two largest terms in Eq. (44) are

$$e^{2\beta(K_2+K_3-|K_1|)}e^{6\beta Ah} - 2e^{2\beta(|K_1|+K_2+K_3)} \approx 0, \quad (47)$$

which reduces to

$$Ah \approx \frac{1}{6}kT \ln 2 + \frac{2}{3}|K_1|. \quad (48)$$

Again the slope of the critical line at $T=0$ is positive. The $T \rightarrow 0$ limit of Ah depends only on the negative coupling coefficient, K_1 .

In the exceptional case when $\gamma_2 > \gamma_3$ and $\gamma_3 = \frac{1}{3}$, Eq. (44) can be rewritten as

$$e^{2\beta(K_2-(2/3)|K_1|)}e^{6\beta Ah} + 2e^{2\beta K_2}e^{4\beta Ah} + e^{2\beta(K_2+(2/3)|K_1|)}e^{2\beta Ah} - 2e^{2\beta(K_2+(4/3)|K_1|)} \approx 0, \quad (49)$$

All four terms of Eq. (49) are equally large. Assuming $\exp(2\beta Ah) = a_1 \exp(\frac{4}{3}\beta|K_1|)$, we obtain

$$Ah \approx \frac{1}{2}kT \ln a_1 + \frac{2}{3}|K_1| \approx -0.181475kT + 2K_3, \quad (50)$$

where $a_1 = \frac{1}{3}[-2 + (1/c_1) + c_1]$ with $c_1 = (28 + \sqrt{783})^{1/3}$.

In the case when $\gamma_2 = \gamma_3$, instead of Eq. (44), we have

$$e^{2\beta(2K_3-|K_1|)}e^{6\beta Ah} + 4e^{2\beta K_3}e^{4\beta Ah} + 4e^{2\beta|K_1|}e^{2\beta Ah} - 2e^{2\beta(|K_1|+2K_3)} \approx 0. \quad (51)$$

Case (ii-c): $\gamma_2 = \gamma_3 < \frac{1}{3}$

Only the last two terms of Eq. (51) are dominant, and we have

$$Ah \approx -\frac{1}{2}kT \ln 2 + 2K_3. \quad (52)$$

Case (ii-d): $\gamma_2 = \gamma_3 > \frac{1}{3}$

Only the first and last terms of Eq. (51) are dominant, and we have Eqs. (47) and (48). That is,

$$Ah \approx \frac{1}{6}kT \ln 2 + \frac{2}{3}|K_1|.$$

However, if $\gamma_2 = \gamma_3 = \frac{1}{3}$, all four terms of Eq. (51) are equally large and we have

$$Ah \approx \frac{1}{2}kT \ln a_2 + 2K_3 \approx -0.511793kT + 2K_3, \quad (53)$$

where $a_2 = \frac{1}{3}[-4 + (4/c_2) + c_2]$, with $c_2 = (35 + \sqrt{1161})^{1/3}$.

Let us find A from the spin configuration of the ground state. The energy is $E = |K_1|\sum_{\langle ij \rangle} s_i s_j - K_2\sum_{\langle ij \rangle} s_i s_j - K_3\sum_{\langle ij \rangle} s_i s_j - h\sum_i s_i$. When h is small, the spin configuration is as shown in Fig. 9(b) (K_1 is the vertical link.) and $E = (-|K_1| - K_2 - K_3)N/2$. This corresponds to an antiferromagnetic state. As h increases, the spin configuration changes into a paramagnetic state [Fig. 9(d)], with a lower energy $E = (|K_1| - K_2 - K_3 - 2h)N/2$. The transition takes place when the energies of the two states become identical, or $h = |K_1|$. We therefore obtain $A = 2K_3/|K_1| = 2\gamma_3$ for the cases (ii-a) and (ii-c) and $A = \frac{2}{3}$ for cases (ii-b) and (ii-d) and the two exceptional cases.

C. Case (iii): $K_1 > 0, K_2 < 0, K_3 < 0$

Rewriting the Ising partition function on an elementary cycle in terms of magnitudes of coupling coefficients, we obtain

$$\begin{aligned} z(T, h) = & e^{2\beta(K_1-|K_2|-|K_3|)}(e^{6\beta h} + e^{-6\beta h}) + 2(e^{2\beta K_1} \\ & + e^{-2\beta|K_2|} + e^{-2\beta|K_3|})(e^{4\beta h} + e^{-4\beta h}) + [2(e^{2\beta K_1} \\ & + e^{2\beta|K_2|} + e^{2\beta|K_3|} + e^{-2\beta K_1} + e^{-2\beta|K_2|} + e^{-2\beta|K_3|}) \\ & + e^{2\beta(K_1+|K_2|+|K_3|)} + e^{-2\beta(K_1+|K_2|-|K_3|)} \\ & + e^{-2\beta(K_1-|K_2|+|K_3|)}](e^{2\beta h} + e^{-2\beta h}) \\ & + 2e^{-2\beta(K_1+|K_2|+|K_3|)} + 2e^{2\beta(K_1+|K_2|-|K_3|)} \\ & + 2e^{2\beta(K_1-|K_2|+|K_3|)} + 4e^{-2\beta K_1} + 4e^{2\beta|K_2|} \\ & + 4e^{2\beta|K_3|} + 2e^{-2\beta(K_1-|K_2|-|K_3|)}. \end{aligned} \quad (54)$$

Making the transformation we obtain the equation for the critical line,

$$\begin{aligned} -e^{2\beta(K_1-|K_2|-|K_3|)}(e^{6\beta f(|h|)} + e^{-6\beta f(|h|)}) + 2(e^{2\beta K_1} \\ - e^{-2\beta|K_2|} - e^{-2\beta|K_3|})(e^{4\beta f(|h|)} + e^{-4\beta f(|h|)}) + [2(e^{2\beta K_1} \\ + e^{2\beta|K_2|} + e^{2\beta|K_3|} - e^{-2\beta K_1} - e^{-2\beta|K_2|} - e^{-2\beta|K_3|}) \\ - e^{2\beta(K_1+|K_2|+|K_3|)} - e^{-2\beta(K_1+|K_2|-|K_3|)} \\ - e^{-2\beta(K_1-|K_2|+|K_3|)}](e^{2\beta f(|h|)} + e^{-2\beta f(|h|)}) \\ + 2e^{-2\beta(K_1+|K_2|+|K_3|)} + 2e^{2\beta(K_1+|K_2|-|K_3|)} \\ + 2e^{2\beta(K_1-|K_2|+|K_3|)} - 4e^{-2\beta K_1} + 4e^{2\beta|K_2|} + 4e^{2\beta|K_3|} \\ + 2e^{-2\beta(K_1-|K_2|-|K_3|)} = 0. \end{aligned} \quad (55)$$

Let us assume $|K_2| \geq |K_3|$ without loss of generality. Let us again define three parameters, $K_1 = K$, $|K_2| = \gamma_2 K$, and $|K_3| = \gamma_3 K$. We made a few plots of Eq. (55) for different combinations of (γ_2, γ_3) . As we see in Fig. 12, the critical line is interesting and complicated in this case. The bulge on the right means that the antiferromagnetic phase transition is possible above the zero-field critical temperature. As the magnetic-field strength is increased, the critical temperature rises, whereas it decreases in cases (i) and (ii). But as the field is increased further $\tau_c(h)$ eventually begins to fall again. This type of behavior was conjectured for a fcc lattice [14] and found in the antiferromagnetic triangular Ising model [16,23]. *In the bulge region the system begins from a disordered state in the zero-field limit. As you increase the field strength the system enters into an antiferromagnetic phase and then into a paramagnetic phase.*

The overall behavior of the critical line is as follows.

(i) The $T \rightarrow 0$ limit of h_c is, for all combinations of (γ_2, γ_3) ,

$$Ah_c = |K_2| + |K_3|. \quad (56)$$

(ii) Case $\gamma_2 = \gamma_3$: below $\gamma_2 \approx 0.6725$ the line starts moving to the up-left direction towards the end point as in the cases (i) and (ii). Above $\gamma_2 \approx 0.6725$ the line veers to the

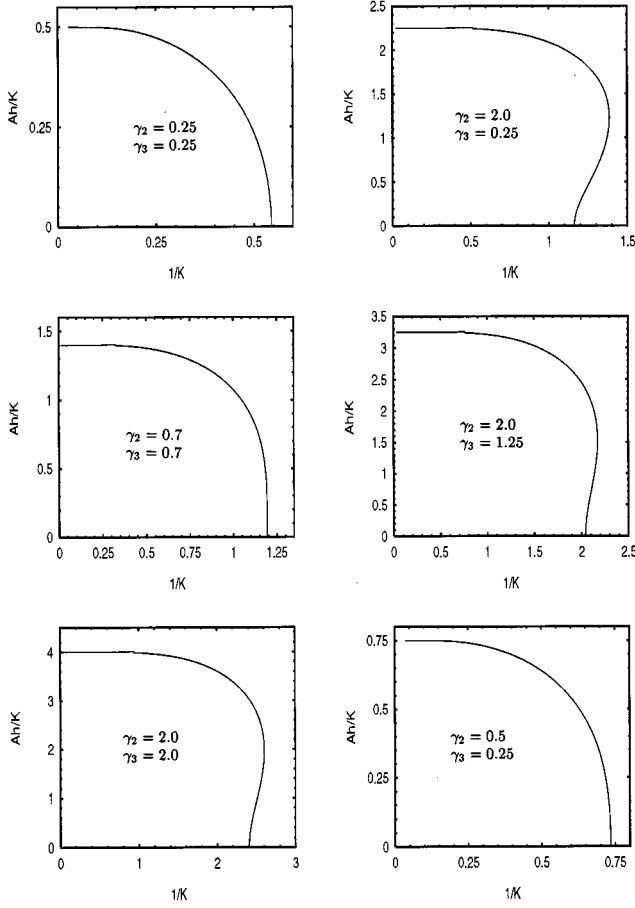


FIG. 12. Critical lines of an Ising antiferromagnet on a honeycomb lattice: $K_1 > 0$, $K_2 < 0$, and $K_3 < 0$.

up-right direction, then turns to left, and rises monotonically up to its final value in the limit $T=0$.

(iii) Case $\gamma_2 \neq \gamma_3$: the line has both behaviors as in the $\gamma_2 = \gamma_3$ case but it is not easy to make compact descriptions. It veers up-right and turns left, or moves up-left from the outset, depending on the values of (γ_2, γ_3) . It is best illustrated in Fig. 13, where the values of $A\eta_b$ and τ_b at the turning points are shown.

We made contour plots of $(\gamma_2, \gamma_3, \tau_c)$, which is again identical to Fig. 7. The contours of $(\gamma_2, \gamma_3, A\eta_b)$ are shown in Fig. 13(a). Along any direction in the γ_2 - γ_3 plane its profile is practically linear with the same slope. The contours of $(\gamma_2, \gamma_3, \tau_b)$ are shown in Fig. 13(b). Along the direction $\gamma_2 = \gamma_3$ it increases very slowly but as you go away from this direction its slope becomes steeper and its profile is close to linear. The bulge appears when the point (γ_2, γ_3) falls outside the nearly circular contour with the value $\tau_b = 1$.

Since $Ah \approx |K_2| + |K_3|$ in the $T \rightarrow 0_+$ limit, the largest terms in Eq. (55) are,

$$\begin{aligned} & -e^{2\beta(K_1 - |K_2| - |K_3|)} e^{6\beta Ah} + 2e^{2\beta K_1} e^{4\beta Ah} \\ & -e^{2\beta(K_1 + |K_2| + |K_3|)} e^{2\beta Ah} + 2e^{2\beta(K_1 + |K_2| - |K_3|)} \approx 0. \end{aligned} \quad (57)$$

or, upon discarding the last term and performing some algebraic manipulations,

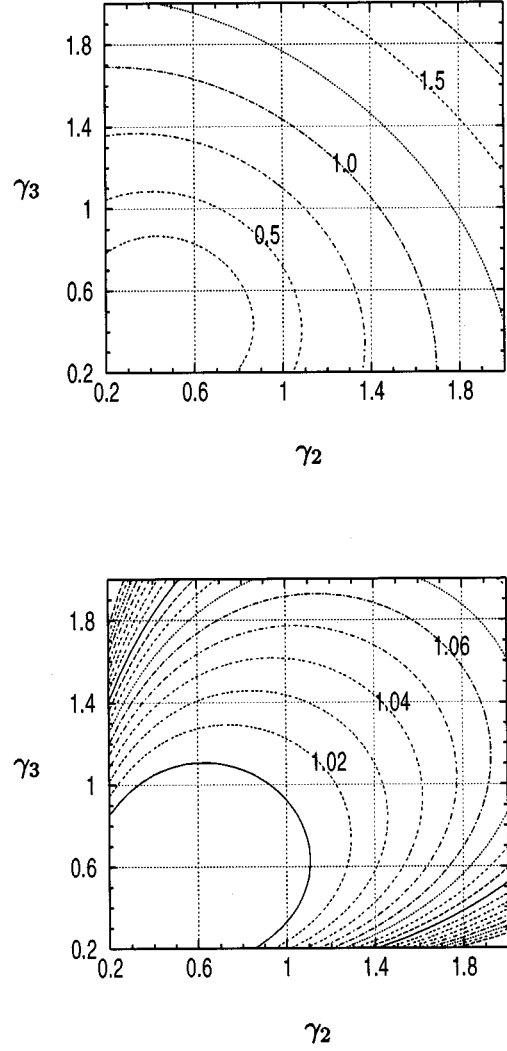


FIG. 13. Bulge locations, $A\eta_b(\gamma_2, \gamma_3)$ and $\tau_b(\gamma_2, \gamma_3)$: $K_1 > 0$, $K_2 < 0$, and $K_3 < 0$.

$$e^{2Ah} \approx e^{2\beta(|K_2| + |K_3|)}, \quad (58)$$

which reduces to

$$Ah \approx (|K_2| + |K_3|). \quad (59)$$

The slope of the critical line at $T=0$ is zero. The $T \rightarrow 0$ limit of Ah depends only on the negative coupling coefficients, K_2 and K_3 .

Let us find A from the ground-state spin configuration. The energy is $E = -K_1 \sum_{\langle ij \rangle} s_i s_j + |K_2| \sum_{\langle ij \rangle} s_i s_j + |K_3| \sum_{\langle ij \rangle} s_i s_j - h \sum_i s_i$. When h is small, the lowest-energy spin configuration is as shown in Fig. 9(c) (K_1 is the vertical link.) and $E = (-K_1 - |K_2| - |K_3|)N/2$. This corresponds to an antiferromagnetic state. As h increases, the spin configuration changes into a paramagnetic state [Fig. 9(d)] with a lower energy $E = (-K_1 + |K_2| + |K_3| - 2h)N/2$. The transition takes place when the energies of the two states become identical or $h = |K_2| + |K_3|$. Thus we obtain $A = 1$.

V. CONCLUSION

In this paper we extended our approach introduced in Ref. [19] to an anisotropic Ising antiferromagnet on square and honeycomb lattices with some or all negative interaction strengths. We proved that the exact zero-field critical conditions of an Ising antiferromagnet are determined by the zeros of the pseudopartition function on an elementary cycle. Using the fact that the critical point of an Ising antiferromagnet corresponds to the singularity of its free energy and the Griffiths' smoothness postulate, we extended our previous conjecture for the case with nonzero magnetic field and obtained the critical lines of an Ising antiferromagnet on these lattices. Our results reasonably agree with the formula obtained by Müller-Hartmann and Zittartz. It will be useful to check our results for the honeycomb lattice by different means such as Monte Carlo simulation or series analysis.

The critical lines are depicted for each different combination of the coupling coefficients. We also made plots of the zero-field critical temperatures of an Ising antiferromagnet on square and honeycomb lattices as functions of the ratios of the coupling coefficients. The low- T limit of the critical line is obtained for each case from the ground-state spin

configurations. We observed two interesting phenomena may occur. In the cases of a square lattice with ($K_1 > 0, K_2 < 0$) and a honeycomb lattice with ($K_1 < 0, K_2 < 0, K_3 < 0$) and ($K_1 < 0, K_2 > 0, K_3 > 0$), the critical line has a positive slope in the zero T limit and thus has a maximum at a temperature $\tau_m \neq 0$, except for some rare cases. This means that for a given magnetic field phase transitions are possible at two different temperatures as disputed in the past and that the antiferromagnet is not necessarily most inert against demagnetizing field at the absolute zero. We have made plots of the temperatures τ_m where the antiferromagnetic system is most inert and the critical fields $A \eta_m$ at τ_m as functions of the ratios of the coupling coefficients. In the case of a honeycomb lattice with ($K_1 > 0, K_2 < 0, K_3 < 0$) a field-driven antiferromagnetic phase transition is possible. We made plots of the maximum temperatures τ_b where the phase transition is possible and the critical fields $A \eta_b$ at τ_b as functions of the ratios of the coupling coefficients.

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