On the BNNNI model in the free-fermion approximation

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Abstract. In the free-fermion approximation, we map the BNNNI model onto the nearest-neighbour Ising model for the general anisotropic case. The resulting phase diagram does not contain floating phases but the transition lines between other phases agree with the earlier studies, which were restricted to the isotropic case.

1. Introduction

Recently much attention has been paid to a frustrated Ising model called the BNNNI (biaxial next-nearest-neighbour Ising) model where each spin (± 1) on a square lattice interacts with its nearest and next-nearest (in both directions) neighbours through the Hamiltonian

$$\mathcal{H} = -\sum_{x,y} s(x, y)(J_{1x}s(x+1, y) + J_{1y}s(x, y+1) + J_{2x}s(x+2, y) + J_{2y}s(x, y+2)) \tag{1}$$

where $s(x, y)$ is the spin at the site (x, y). The phase diagram consists of paramagnetic ferromagnetic, antiphase and, perhaps, an incommensurate phase. In the special case of isotropic interaction $J_{1x} = J_{1y} = J_1$ (say) and $J_{2x} = J_{2y} = J_2$ (say), previous works have determined the phase diagram (figure 1) by various methods such as Monte Carlo [1-5], renormalization group [1, 6, 7], and high- and low-temperature series expansion [8]; the presence of an incommensurate phase has been excluded by some of the studies [1, 4] and supported by some others [2, 5, 6]. To our knowledge, the anisotropic case has not been treated so far.

In this paper, we present an analysis of the phase diagram for the general (anisotropic) case $J_{1x} \neq J_{1y}$, $J_{2x} \neq J_{2y}$ in the free-fermion approximation. This approximation has been found to be quite reasonable for the ANNNI model (in two dimensions) [9, 10] and has not yet been applied to the BNNNI model until now. We have shown elsewhere [11] that using a general form of the free-fermion approximation the phase diagram of the two-dimensional ANNNI model can be easily and accurately determined by a mapping onto the standard (nearest-neighbour) Ising model although the incommensurate ('floating') phase cannot be obtained. Here we shall follow that approach to obtain the phase diagram (which agrees reasonably well with the previous studies) of the BNNNI model, remembering that we are unable to treat the crucial issue of the presence of an incommensurate phase. In section 2 we shall derive the expressions for the critical lines and in section 3 we shall discuss the phase diagram so obtained.
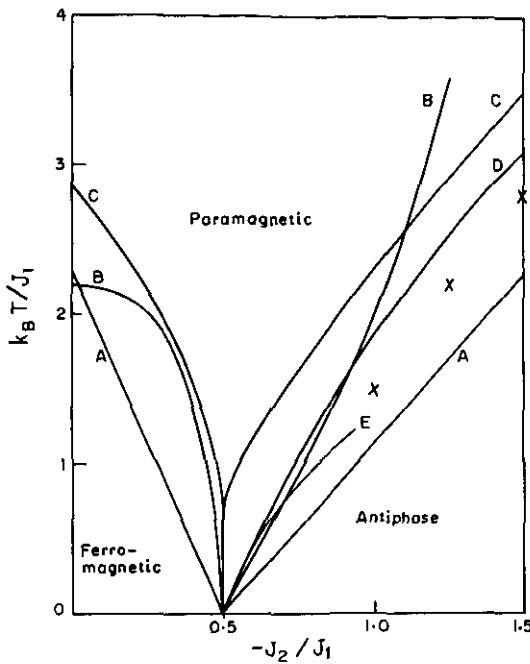
Figure 1. Phase diagram for the isotropic case. The doubtful presence of an incommensurate phase is not shown. A, present study; B, [5]; C, [6]; D, [8]; E, [2]; crosses, [4]. For the region $0 > (J_2/J_1) > 0.5$, the results of [2, 7, 8] more or less coincide with A and are not therefore shown separately.

2. Derivation of the expressions for critical temperature

The precise form of the free-fermion approximation that we shall use is the following: (i) In the BNNNI model there is no antiferromagnetic domain, i.e. the separation of domain walls (on the dual lattice) is always greater than unity. (We shall call this the no antiferromagnetic domain (NAF) approximation.) (ii) In the standard (nearest-neighbour) Ising model single (isolated) spin flips are excluded. (This is equivalent to the NAF approximation for the ferromagnetic ground state.) Also, let $K_x = J_{1x} + 2J_{2x}$, $K_y = J_{1y} + 2J_{2y}$.

Case I: $K_x > 0$, $K_y > 0$

In this case we have, following [11], a one-to-one mapping between the free energies of the BNNNI model and the standard model:

$$F_B(J_{1x}, J_{1y}, J_{2x}, J_{2y}, T) = F_S(K_x, K_y, T) + (J_{2x} + J_{2y})N \qquad (2)$$

where N is the total number of spins. From the standard expression for critical temperature in the Onsager solution (see equation (7.12.8) of [12]) one immediately obtains the expression for the critical temperature T_c in the BNNNI model:

$$\sinh(2\beta K_x) \sinh(2\beta K_y) = 1 \qquad (3)$$

where $\beta = 1/k_B T_c$ and k_B is the Boltzmann constant. The basic idea behind the derivation of (2) is that if the domain walls are of total length H in the X-direction

and V in the Y-direction, then one can write down the free energies F_B and F_S in terms of H and V and both sides of (2) are equal to

$$-J_{1x}(N-2V)-J_{1y}(N-2H)-J_{2x}(N-4V)-J_{2y}(N-4H)$$
$$-k_B T \ln \Omega(K_x V + K_y H). \tag{4}$$

(Here, $\Omega(E)$ is the total number of microstates with a given value of E.) However, this argument is true only for $K_x > 0$ and $K_y > 0$, since otherwise the NAF assumption, although true for the BNNNI model, goes wrong for nearest-neighbour model as the antiferromagnetic phase becomes the ground state.

Case II: $K_x < 0$, $K_y < 0$

Here the ground state of the BNNNI model is the antiphase state ('chessboard' or 'staircase' configuration of [8]). Now we shall map this model onto a slightly modified version of the standard model. Thus, following [11], we break up the lattice into two sublattices $\mathscr{L}_1$ (for which $x+y$ = odd integer) and $\mathscr{L}_2$ (for which $x+y$ = even integer) and impose nearest-neighbour antiferromagnetic interactions on each of them. The Hamiltonian for the whole system is then

$$\mathscr{H}_N = -\sum_{x,y} s(x, y)(J'_x s(x+2, y) + J'_y s(x, y+2)) \tag{5}$$

where J'_x, J'_y are both negative. Now, the antiferromagnetic ground state of $\mathscr{L}_1$ and $\mathscr{L}_2$ constitutes the antiphase ground state of the whole system and the NAF assumption on $\mathscr{L}_1 + \mathscr{L}_2$ is equivalent to the exclusion of single (isolated) spin flip in the antiferromagnetic state of $\mathscr{L}_1$ and of $\mathscr{L}_2$. The free energy in this approximation is therefore given by

$$F_N(J'_x, J'_y, T) = -J'_x(N-4V) - J'_y(N-4H) - k_B T \ln \Omega(J'_x V + J'_y H). \tag{6}$$

A comparison with expression (4) leads to the mapping

$$F_B(J_{1x}, J_{1y}, J_{2x}, J_{2y}) = F_N(K_x/2, K_y/2, T) + (J_{2x} + J_{2y})N. \tag{7}$$

Since the free energy and critical temperature of both the lattices $\mathscr{L}_1$ and $\mathscr{L}_2$ (and hence of the whole system $\mathscr{L}_1 + \mathscr{L}_2$) is given by the usual Onsager expressions, one obtains the expression for the critical temperature as

$$\sinh(\beta K_x) \sinh(\beta K_y) = 1. \tag{8}$$

Case III: $K_x K_y < 0$

The extension to the case $K_x > 0$ but $K_y < 0$ is straightforward. Following the above procedure for free energy $F_{N^{+-}}(J_x, J'_y, T)$ of the Hamiltonian

$$\mathscr{H}_{N^{+-}} = -\sum_{xy} s(x, y)(J_x s(x+1, y) + J'_y s(x, y+2)) \tag{9}$$

can be related to the free energy of the BNNNI model:

$$F_B(J_{1x}, J_{1y}, J_{2x}, J_{2y}, T) = F_{N^{+-}}(K_x, K_y/2, T) + (J_{2x} + J_{2y})N. \tag{10}$$

The crucial temperature is obviously given by

$$\sinh(2\beta K_x) \sinh(\beta K_y) = -1. \tag{11}$$

Similarly one may obtain the critical line for the case $K_x < 0$ but $K_y > 0$. Combining all the results the critical line is, in general, given by

$$\sinh[(3+\text{sgn } K_x)\beta K_x/2]\sinh[(3+\text{sgn } K_y)\beta K_y/2] = \pm 1 \qquad (12)$$

whatever the sign of K_x and K_y. Here $\text{sgn}(x)$ is the sign function ($+1$ for $x>0$, -1 for $x<0$, 0 for $x=0$).

3. Results for the different cases

The phase diagram will always consist of ferromagnetic, paramagnetic and antiphase states and is presented in figure 2 for the anisotropic case. However, the ground state depends on the sign of K_x and K_y. For $K_i > 0$ (<0), there is ferromagnetic (antiphase) order in the direction i ($i = X$ or Y).
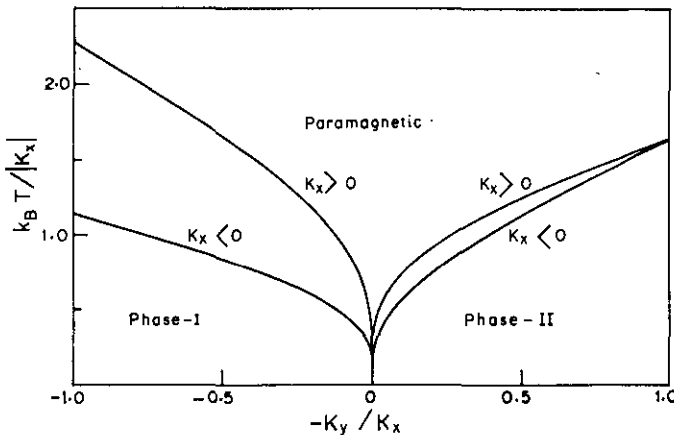

Figure 2. Phase diagram for the anisotropic case. $K_x = J_{1x} + 2J_{2x}$, $K_y = J_{1y} + 2J_{2y}$. For $K_x > 0$, phase I is the normal ferromagnetic phase and phase II is a phase (denoted by (F, AP)) that possesses ferromagnetic order in the X-direction and antiphase order in the Y-direction. For $K_x < 0$, phase I is (AP, AP) and phase II is (AP, F).

For the special case of isotropic interaction, i.e. $J_{1x} = J_{1y} = J_1$ and $J_{2x} = J_{2y} = J_2$, the above equations (3) and (8) for critical temperature become

$$k_B T_c/J_1 = [2+4(J_2/J_1)]/\log(\sqrt{2}+1) \qquad \text{for } J_1 + 2J_2 > 0$$

$$= [1+2(J_2/J_1)]/\log(\sqrt{2}-1) \qquad \text{for } J_1 + 2J_2 < 0. \qquad (13)$$

As in [11] these expressions are identical with those obtained by the Muller–Hartmann–Zittartz approximation [1]. This result is compared with other approximate results in figure 1 where the agreement is found to be reasonable.

A comment is in order. As in [11] the absence of a phase transition for $K_x = 0$ or $K_y = 0$ arises easily from the above treatment, since the system then reduces to a one-dimensional Ising chain according to (2), (7) and (10).

Let us now discuss the basic approximation involved in this treatment. Apart from making the NAF assumption we have overestimated the entropy (pretended that some configurations (in the standard Ising model) which actually violate the NAF assumption

do satisfy it). In an exact treatment one should assume that there are in general some pairs of sites (in the dual lattice) where the domain walls *are* separated by unit distance along the X and Y axis; let their numbers be p_1 and p_2 respectively. Following [11] it is easy to see that the *exact* expression for the free energy now becomes

$$F_B(J_{1x}, J_{1y}, J_{2x}, J_{2y}, T) = -J_{1x}(N - 2V) - J_{1y}(N - 2H) - J_{2x}[N - 4(V - p_1)]$$

$$- J_{2y}[N - 4(H - p_2)] - k_B T \ln \Omega(K_x V + K_y H - 2J_{2x}p_1 - 2J_{2y}p_2). \qquad (14)$$

For $J_{2x}, J_{2y} \gg T$, the entropy term is small and there is effectively a repulsion between the domain walls when (and only when) they are at unit distance. This justifies the NAF assumption for the BNNNI model. However, there is no such interaction in any case in the nearest-neighbour Ising model and the NAF assumption is reasonable only for $K_x, K_y \gg T$, when the total lengths H, V themselves are small. Thus, our treatment is more reliable at low temperatures and it is this uncertainty that prevents us from conclusively excluding the presence of an incommensurate phase.

Moreover, as in [11], the NAF assumption seems to be very much in error in the three-dimensional nearest-neighbour Ising model. This is because one can immediately apply the above treatment to the three-dimensional isotropic model with nearest- and next-nearest-neighbour interaction and the resulting phase diagram turns out to be topologically the same as that for two dimensions (i.e. figure 1) and this is obviously in contradiction with the present belief [13].

Lastly, a few words about the *disorder line*, i.e. the line across which the correlation (in the paramagnetic phase) changes from oscillatorily decaying to monotonically decaying [1, 9]. Obviously, according to the present mapping the correlation is monotonically (oscillatorily) decaying in both the directions when K_x and K_y are positive (negative). Thus, in the isotropic case (figure 1) the disorder line is a line parallel to the temperature axis and passing through the point $-J_2/J_1 = 0.5$. (Actually, the treatment of [11] predicts the same disorder line there also.)

In conclusion, we have presented here a mapping of the BNNNI model onto the nearest-neighbour Ising model for the general (anisotropic) case in the free-fermion approximation. This provides a simple physical picture and for the isotropic case gives incidentally the same phase diagram as obtained by the Muller–Hartmann–Zittartz method.

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