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LETTER TO THE EDITOR

Phase transition lines via surface energy calculations in the two-dimensional ANNNI model

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Abstract. Using the method of Müller-Hartmann and Zittartz, we calculate the phase transitions of the low-temperature phases of the ANNNI model. The results are confirmed by numerical calculations.

Recently the axial next-nearest-neighbour interaction Ising (ANNNI) model has attracted considerable interest (Hornreich *et al* 1979, Selke and Fisher 1980, Villain and Bak 1981, Selke 1981, which contains a lot of further references). It appears to be the simplest model exhibiting spatially modulated phases. In this note the method of Müller-Hartmann and Zittartz (1977; in the following referred to as MHZ) is applied to the two-dimensional ANNNI model and the transition lines corresponding to the melting of the two low-temperature phases (ferromagnetic and (2,2) structure) are determined within this method.

The two-dimensional ANNNI model is characterised by the Hamiltonian

$$H = -\sum_{i,j} (J_\perp S_{i,j}S_{i+1,j} + J_1 S_{i,j}S_{i,j+1} - J_2 S_{i,j}S_{i,j+2}),$$

$$S_{i,j} = \pm 1, \qquad J_\perp, J_1 > 0, \qquad -M+1 \leqslant i \leqslant M, \qquad -N+1 \leqslant j \leqslant N. \quad (1)$$

In this Letter we discuss separately the cases $J_2/J_1 < 0.5$, where one has a ferromagnetically ordered low-temperature phase, and $J_2/J_1 > 0.5$, where a so-called (2,2) structure (two spins up, two spins down in a row) is favoured. For the special cases $J_1 = 0$ or $J_2 = 0$ (nearest-neighbour Ising model) the properties of the above model are known exactly.

In the following we calculate the free energy σ of an interface between two regions with either different ferromagnetic or different (2,2) states. Phase transitions are then indicated by a zero of σ. MHZ assume that it is sufficient to take into account only simple non-reversing interfaces. In spite of this restriction, the results are often satisfactory, in some cases even exact (Burkhardt 1978, Lin and Wu 1979, Zittartz 1981).

(a) $J_2/J_1 > 0.05$

For $J_2/J_1 > 0.5$ we have chosen the arrangement shown in figure 1. The shape of the interface is characterised by the integers m_k, n_k ($-M+1 \leqslant m_k, n_k \leqslant M$), which denote the position of the interface in the columns $2k$ and $2k+1$, respectively. The assumption of only one simple interface from left to right in the MHZ method appears to be justified

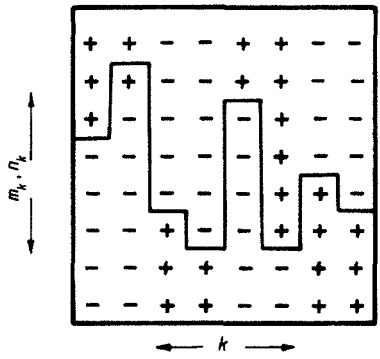

Figure 1. A typical configuration with one interface for $J_2/J_1 > 0.5$. The two spin directions are represented by + and −. The columns are numbered by k. The position of the interface in the columns $2k$ and $2k+1$ are denoted by m_k and n_k, respectively.

in particular for large $J_\perp$ (Hamiltonian limit). In the thermodynamic limit the interface energy σ is given by

$$\sigma = -k_B T \lim_{N\to\infty} \frac{1}{2N} \ln \sum_{\{m_k, n_k\}} \exp(-\Delta E/k_B T) \tag{2}$$

with

$$\Delta E = 4NJ_\perp + \sum_{k=1}^{N} (-2J_1|m_k - n_k| + 2J_1|n_k - m_{k+1}| + 2J_2|m_k - m_{k+1}| + 2J_2|n_k - n_{k+1}|).$$

The sum over all configurations in (2) can be performed with the help of a corresponding transfer matrix P. From the largest eigenvalue, λ_{max}, of P we determine the phase boundary as usual ($K_\perp = J_\perp/k_B T$):

$$\sigma = 2K_\perp - \tfrac{1}{2} \ln \lambda_{max} = 0 \qquad \text{for } T = T_c. \tag{3}$$

In our case the transfer matrix P is given by

$$P(m, n; m', n') = \exp[2K_1(|n-m| - |n-m'|) - 2K_2(|m-m'| + |n-n'|)]$$

with

$$K_i = J_i/k_B T, \qquad i = 1, 2. \tag{4}$$

In comparison with former applications of the MHZ method, the eigenvalue problem based on (4) looks more involved because of the double indices (m, n). As a first simplification we observe that the eigenvectors of P can be written in the form

$$f(m, n) = \exp[iq(m+n)]g(m-n). \tag{5}$$

On account of the positivity and symmetry of the operator P, the eigenvector corresponding to λ_{max} must be positive and symmetric (Perron–Frobenius theorem), allowing only $q = 0$ in (5). Introducing the difference variable $u = m - n$, the eigenvalue problem is thus reduced to the form

$$\lambda_{max} g(|u|) = \sum_{v=-\infty}^{\infty} V(u, v) g(|v|). \tag{6}$$

One finds that in the limit $u \to \infty$ the operator V as calculated from P becomes a difference kernel $\bar{V}(u-v)$ up to exponential corrections $O[\exp(K_1-2K_2)u]$:

$$\bar{V}(u-v) = y_+ \exp[-(2K_2+K_1)|v-u|] - y_- \exp[-(2K_2-K_1)|v-u|],$$
$$y_\pm = 1/[\exp(2K_1 \pm 4K_2)-1] - 1/[\exp(2K_1)-1]. \tag{7}$$

Consequently, as the eigenvalues of V and $\bar{V}$ are the same, we have

$$\lambda_{\max} = \sum_{u=-\infty}^{\infty} \bar{V}(u). \tag{8}$$

From (3) we obtain the transition line of the (2, 2) region:

$$2K_\perp = \ln\{(1-\exp(-4K_2))/[(1-\exp(-K_1-2K_2))(1-\exp(K_1-2K_2))]\}. \tag{9}$$

For $K_1 = 0$ equation (9) contains the correct transition line of the ordinary Ising model. In addition we have calculated numerically the maxima of the specific heat of the ANNNI model for a $12 \times \infty$ strip. Here the transfer matrix connecting neighbouring rows was used to determine the bulk free energy. The agreement with our analytical calculations is very satisfactory (see figure 2). Furthermore our result is nicely confirmed by Monte Carlo simulations (Selke 1981). In our analytic calculation we have only considered the interface generated by the combination of states shown in figure 1. Due to the fourfold degeneracy of the (2, 2) phase, there exists another combination of states, the interface of which, however, leads to a lower $\lambda_{\max}$ and therefore to a higher transition temperature.

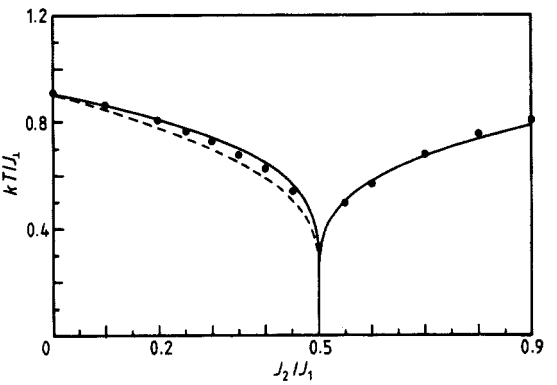

Figure 2. The full line represents the phase transition, calculated by our application of the MHZ method. The broken line is obtained from equation (10). The circles correspond to maxima of the specific heat in a $12 \times \infty$ strip ($J_\perp/J_1 = 10$).

(b) $J_2/J_1 < 0.5$

Similar considerations can be applies to the ferromagnetic side ($J_2/J_1 < 0.5$) using the geometry of figure 1, but with competing ferromagnetic configurations separated by the interface. Unfortunately, the corresponding eigenvalue $\lambda_{\max}$ could be evaluated analytically only for $J_2 = 0$ and for $J_2/J_1 \to -\infty$, where the exact expression for the transition point is recovered. For general values of J_2, we have calculated $\lambda_{\max}$ numerically and thereby the transition line. In the interval $0 \leq J_2/J_1 < 0.5$ the result deviates slightly

from an analytical expression given by Hornreich *et al* (1979):

$$\sinh(K_\perp)\sinh(2K_1 - 4K_2) = 1. \tag{10}$$

The relation (10) was derived arranging the interface perpendicular to the direction of $J_\perp$. In this case one can proceed in complete analogy to the original calculation of MHZ by substituting $K_1 \to K_1 - 2K_2$ there. Equation (10), too, reproduces the exact transition point for $J_2 = 0$ and for the multicritical point $J_2/J_1 = 0.5$, but in contrast to our approach it fails for $J_2/J_1 \to -\infty$. Nevertheless equation (10) must be considered as a fine analytical description of the transition line in the interval $0 \leqslant J_2/J_1 < 0.5$ (Selke 1981). In figure 2 we have compared our result with equation (10) and the maxima of the specific heat obtained as described before.

In summary, we have shown that the two low-temperature transition lines can apparently be described analytically for $0 \leqslant J_2/J_1 < \infty$ by equations (9) and (10) very accurately. Furthermore, we conclude that the MHZ method is not *a priori* confined to situations with only two degenerate ground-state configurations, as it has been supposed before (Lin and Wu 1979).

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