Mean-Field Axial Next-Nearest-Neighbor Ising Model with an Arbitrary Intralayer Interaction

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We study the mean-field version of the axial next-nearest-neighbor Ising (ANNNI) model with an arbitrary intralayer coupling. Within the mean-field theory there is the possibility of emergence of commensurate phases with the same period but with different symmetries. We study the transition between these different types of commensurate phases as a function of the intralayer coupling. We also study the dependence of the accumulation points on the strength of the intralayer coupling.

I. Introduction

The axial next-nearest-neighbor Ising, or ANNNI model, is one of the simplest models exhibiting modulated structures. In this model each spin $S_i = \pm 1$ interacts with nearest-neighbor coupling $J_1 > 0$ and next-nearest-neighbor coupling J_2 along one lattice direction, and with nearest-neighbor ferromagnetic coupling $J_0 > 0$ within the layers perpendicular to the axial direction. The ANNNI model has been actively studied during the past decade and the subject has matured to the point of receiving two extensive reviews[1,2]. However the model presents a very rich behavior and many of its aspects remain to be explored.

Recently the mean-field phase diagram of the ANNNI model was investigated for arbitrary intralayer interaction J_0 [3,4], thus extending the previous works mostly limited to the case $J_0 = J_1$. The main motivation in carrying out this kind of study was to investigate to what extent the generic aspects of the phase diagram of the ANNNI model is sensitive to the variation of J_0. Interestingly enough, it was observed that some qualitative changes in the phase diagram is brought about by the decrease of J_0, most notably the pinching of some of the commensurate phases, as can be seem in figure 1 showing the phase diagram for $J_0 = 0.2J_1$. The pinching effect is intimately related to the appearance of commensurate structures with disordered (zero magnetization) layers and also of commensurate structures without definite symmetries.

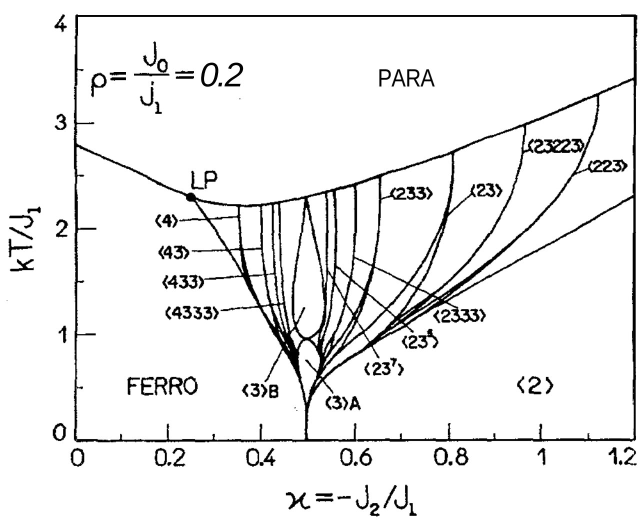

Figure 1. Global phase diagram of the mean-field ANNNI model for $J_0 = 0.2\,J_1$.

In this paper we wish to reexamine the above mentioned effects in greater detail and also to investigate other aspects of the problem left out by previous works. All the calculations will be carried out within the conventional mean-field approximation. Although the mean-field theory of the ANNNI model for $J_0 = J_1$ has revealed to be extremely successful in predicting the qualitative features of the phase diagram, there are no grounds for supposing that the same situation holds for $J_0 < J_1$. In fact, very recent results based on improved mean-field approximation, where the model is treated exactly along the axial direction of competing interactions[5] and Monte Carlo simulations[6] provide strong evidence against the existence of commensurate phases with disordered planes in the *real* ANNNI model. Therefore it is possible that some of the results presented in this paper, in particular those which assume the existence of commensurate phases with disordered planes, will riot be realized in the real ANNNI model, but rather reflect the mathematical properties of the mean-field equations of the ANNNI model. However the disappearance of the accumulation points occurs for rather high value of J_0, namely $J_0 < 0.75J_1$, and may be relevant to the real ANNNI model.

II. Mean-field equations

The free-energy functional of the ANNNI model in the mean-field approximation is given by (see, *e.* g., Ref. [7]),

$$\begin{aligned} N^{-2}F &= -Nk_BT\ln 2 - J_1\sum_n(2\rho M_n^2 \\ &+ M_nM_{n+1} - \kappa M_nM_{n+2}) \\ &+ k_BT\sum_n\int_0^{M_n}\tanh^{-1} m\, dm\,, \end{aligned} \quad (1)$$

where $\rho = J_0/J_1$, $\kappa = -J_2/J_1$, M_n is the magnetization per spin in the nth layer, and N^3 is the number of spins in the system. In what follows we will adopt the unit system such that $k_B = 1$ and $J_1 = 1$. The condition that F be an extremum with respect to M_n gives

$$\begin{aligned} M_n &= \tanh\frac{1}{T}[4\rho M_n + M_{n-1} \\ &+ M_{n+1} - \kappa(M_{n-2} + M_{n+2})]\,. \end{aligned} \quad (2)$$

To be physically acceptable, an extremum should at least be metastable, that is, a local minimum of F. For a given periodic solution of period Q to be a local minimum it is necessary that the matrix

$$M = \prod_{n=1}^{Q}\begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ -1 & \frac{1}{\kappa} & B_n & \frac{1}{\kappa} \end{pmatrix}, \quad (3)$$

where

$$B_n = \frac{1}{\kappa}(4\rho - \frac{T}{1-M_n^2})\,, \quad (4)$$

has no complex eigenvalues of unit modulus[8,9]. Due to the fact that the matrix M is symplectic, the secular equation becomes

$$\lambda^4 - (\mathrm{tr}\, M)\lambda^3 + (\mathrm{tr}_2\, M)\lambda^2 - (\mathrm{tr}\, M)X + 1 = 0\,. \quad (5)$$

This is a reciprocal equation which can easily be solved in terms of quadratic equations.

III. Phase transitions within commensurate phases

When $J_0 < J_1$, that is $\rho < 1$, there is the possibility of phase transitions between commensurate phases with same period but different symmetries. Conventional commensurate phases, those found for $\rho = 1$, will be called of type A and are characterized by the fact that the centers of inversion symmetry are located midway between two planes. Commensurate phases with disordered planes, which can be found for $\rho < 1$, will be called of type B and have the centers of inversion symmetry located on the planes. Finally, commensurate phases with no centers of symmetry of any kind will be called of type C, and usually are present between commensurate phases of types A and B. In this section we study numerically the existence and dependence of these phases on the parameter p. In particular we determine the critical value $\rho_c(q)$, for a given commensurate phase q, such that for $\rho < \rho_c(q)$ there is the possibility of type B and C phases. We remark that in this paper q denotes the reciprocal of wavelength or wavenumber divided by 2π.

The commensurate $q = 1/6$ phase shows the most pronounced effect as the parameter p is varied and it is the easiest to study. Figure 2 shows, for $\kappa = 0.5$, the relative dominance of different types of commensurate $1/6$ phase as a function of the parameter ρ in the T *versus* ρ plane. The transition lines T_A and T_B between A, B and C phases are of second order[11], and were determined by monitoring the eigenvalues of the secular equation (??). In this case we found numerically $\rho_c(1/6) = 0.3$ in agreement with analytical calculations[3]. Notice that as p decreases below 0.3 the B-phase becomes increasingly dominant until at T = 0 it dominates completely. Of course this is an artifact of the mean-field approximation, since for p = 0 the model reduces to a set of non-interacting chains, which has no ordered phase. The C-phase, on the other hand,

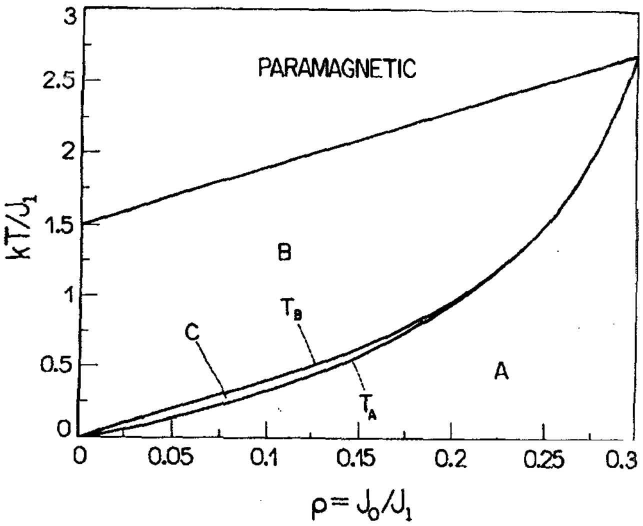

Figure 2. Transition temperatures between different types of commensurate (3) or q = 1/6 phases for $\kappa = 0.5$ in the T *versus* p plane.

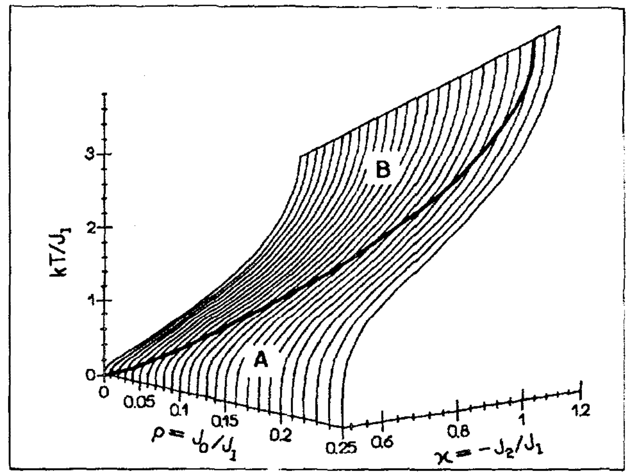

Figure 4. Graph of $\overline{\kappa}$ as a function ot temperature for different values of p for 3/14 phase. The bold line indicates the transition between different types of commensurate q = 3/14 phases.

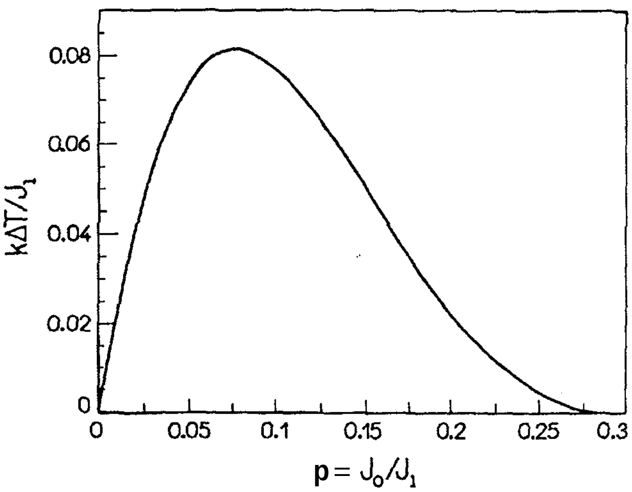

Figure 3. Width of the 1/6 C-phase as a function of p for $\kappa = 0.5$.

first increases tor decreasing ρ and then decreases again to zero for $T = 0$, as shown in Figure 3.

The study of commensurate phases other than $q = 1/6$ is more difficult not only because the widths of commensurate phases are narrower but also because they are slanted relative to the T axis. Let us denote by

$$\overline{\kappa}(T) = \frac{\kappa_l(T) + \kappa_r(T)}{2} , \qquad (6)$$

the average value of κ between the left (κ_l) and right (κ_r) boundaries of the 3/14 phase. The line $\overline{\kappa}(T)$ follows the middle of the 3/14 phase and is equivalent to the line $\kappa = 0.5$ for the 1/6 phase. Figure 4 shows the curves $\overline{\kappa}(T)$ for different values of the parameter p. The heavy line indicates the transition between the A and B phases. The phase C is also present but it is too narrow to be indicated at the scale of the figure. By extrapolating the curve of figure 4 we found numerically that the phase B exists only below $\rho = \rho_c(3/14) = 0.2316\ldots$. In a similar way we have also studied the commensurate phases 1/8 and 1/10. We found numerically $\rho_c(1/8) = 0.2095\ldots$ and $\rho_c(1/10) = 0.1904\ldots$.

Nakanishi[3] provides an analytic expression for $\rho_c(q)$ which gives the results $\rho_c(3/14) = 0.2867\ldots$, $\rho_c(1/8) = 0.2352\ldots$ and $\rho_c(1/10) = 0.2050\ldots$. We tend to attribute the discrepancies between the numerical and analytical calculations of $\rho_c(q)$, except for $q = 1/6$, to the neglect of higher order harmonic terms in the analytical calculations carried out by Nakanishi. In fact, we performed an analytical calculation taking into account up to the eighth harmonic in the expansion of the magnetization and found

$$\rho_c(1/8) = \frac{\sqrt{2}}{20}\left(1 + 6\sqrt{\frac{3}{28}}\right) = 0.2095836\ldots, \qquad (7)$$

in full agreement with numerical calculations.

IV. Evolution of the accumulation points

The transition between cornmensurate phases or between commensurate and incommensurate phases in the ANNNI model can be described by the mechanism of creation of defects (also called walls, discommensurations or solitons)[10]. To be specific, let us consider the phase q = 1/6. At low temperatures the right boundary of the phase 1/6 is composed of segments of first-order transition lines to the phases of the form $\langle 23^j \rangle$. As the temperature increases the segments become shorter and they pile up as $j \to \infty$ at the accumulation point corresponding to the temperature $T_a^r(\rho = 1) = 2.8563\ldots$ [11,12]. Above this temperature the 1/6 phasr undergoes a continuous commensurate-incommensurate transition. Thus the accumulation point separates the boundary composed of first-order transition lines from the boundary consisting of continuou~comrnensurate-incommensurate transition. A similar behavior is found also in the left boundary, the transition being to the phases of the form $\langle 43^j \rangle$ and the accumulation point corresponding to a different temperature $T_a^l(\rho)$. It should be remarked that the transitions to the phases (433) may be cut short by the intervening ferromagnetic phase and have no real existente.

The simplest way to locate the accumulation points is to use the fact that the eigenvalues of the matrix **M** in the phase 1/6, given by the solutions of equation (??), chimge from complex to real, which is related to the cliange over of the interaction between defects at large distances[12]. Figure 5 shows the dependente of $T_a^r(\rho)$ and $T_a^l(\rho)$ on the parameter ρ for the phase **(3)**. The most interesting aspect of these curves is that they tend to zero simultaneously for $\rho = 0.75$, indicating that for $\rho < 0.75$ all the boundaries of the phase 1/6 consist of lines of continuous commensurate-incormnensurate transitions. **A** similar behavior is observed for the phases of the form $\langle 2^j 3 \rangle$. The dependence of $T_a^r(\rho)$ for the cases **j** = 1 and **j** = 2 are also shown in figure 5. At low temperatures it is possible to show that these curves behave as

$$\rho_{\langle 2^j 3 \rangle} \approx \frac{3}{4} - \frac{T}{8} \ln \left[\frac{T}{2(j+1)^2} \right] , \tag{8}$$

thus confirming the numerical result that $\rho \to 3/4$ as $T \to 0$. This iridicates that all the phases $\langle 2^j 3 \rangle$ undergo a second order commensurate-incommensurate transition for $\rho < 3/4$.

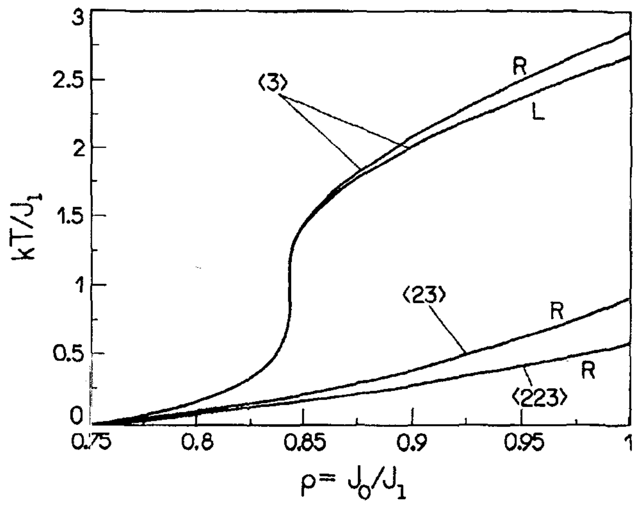

Figure 5. Temperatures of the right (R) and left (L) accumulation points of the (3) or 1/6 phase as a function of the parameter ρ. Also shown are the temperatures of the right accumulation points of the phases (23) and $\langle 2^2 3 \rangle$.

V. Concluding remarks

We investigated two aspects of the mean-field theory of the ANNNI model when the intralayer interaction J_0 is weakened relative to the interlayer interaction J_1. The first aspect is the occurrence of phases with disordered planes. We obtained numerically various values of $\rho(q) = J_0/J_1$ below which disordered phases appear, checking the previous analytical calculations by Nakanishi[3]. The values of $\rho_c(q)$ are, however, rather small, and in the light of recent results[5,6], it is likely that these phases are artifacts of the mean-field approximation and have no counterpart in the real ANNNI model. The second aspect we have investigated concerns the dependence of the location of the accumulation points on the parameter $\rho(q) = J_0/J_1$. For the phases of the form $\langle 2^j 3 \rangle$ we determined numerically as well analytically, that the accumulation points disappear below $\rho = 3/4$, indicating that all the boundaries of these phases become second order.

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