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New Mean-Field Calculations for the Phase Diagram of the Annni Model

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Abstract We use a variational procedure, with the inclusion of some spin fluctuations, to go beyond the standard layer-by-layer mean-field calculations for the T-p phase diagram of the ANNNI model. The high temperature region is studied analytically. The transition lines meet smoothly at the Lifshitz point, which is an inflection point of the second-order paramagnetic border. At low temperatures, our numerical results confirm the stability of the main commensurate phases and show a quantitative trend towards the predictions of the Monte Carlo analyses.

1 INTRODUCTION

In this work we consider one of the simplest spin models to explain the occurrence of complex modulated structures in magnetic compounds. The axial next-nearest-neighbor Ising (or ANNNI) model, proposed by Elliott to account for the magnetic phases of Erbium[1], is defined by the hamiltonian

$$H = \sum_{x,y,z} \left[- J_0 \, S_{x,y,z} \left(S_{x+1,y,z} + S_{x,y+1,z} \right) - J_1 \, S_{x,y,z} \, S_{x,y,z+1} - J_2 \, S_{x,y,z} \, S_{x,y,z+2} \right] - H \sum_{x,y,z} S_{x,y,z} , \tag{1.1}$$

where $S_{x,y,z}$ is an Ising spin (± 1) on the (x,y,z) site of a cubic lattice with unit lattice parameter, The interactions between first neighbors are ferromagnetic (J_0, $J_1 > 0$), while the interactions between second neighbors along the z direction favor an antiferromagnetic alignment ($J_2 < 0$). This axial competition between ferro and antiferromagnetism gives rise to a Lifshitz point and a succession of modulated

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phases[2].

The T-p phase diagram of the ANNNI model, where T is the absolute temperature and $p \equiv -J_2/J_1$ is the ratio of the competing exchange interactions, has been studied by a variety of techniques. In fig. 1 we depict the phase diagram obtained by von Bsehm and Bak[3] within the framework of a careful layer-by-layer mean-field calculation.The analysis of high-temperature series expansions confirms the existence of two distinct paramagnetic lines, at somewhat lower temperatures, which join çmoothly at the Lifçhitm point[4]. However, this sort of analysis gives no indication about the nature of the ordered regions of the phase diagram. Low-temperature series expansions were obtained by Fisher and Selke[S],but are restricted to the asymptotic region near the multiphase point (T = 0; p = 1/21. The analysis of the low-temperature series shows theexistence of a succession of modulated phases springing from the multiphase point, in agreement with the mean-field calculations. Also, detailed numerical studies of the ANNNI model by Monte Carlo techniques have been carried out by Selke and Fisher[6]. From tha qualitative point of view, the available Monte Carlo data agree with the results of the layer-by-layer mean -field calculations and strongly support the existence of modulated phases characterized by well-defined values sf a principal wave number. However, there are some quantitative discrepancies, which still give room for more refined mean-field studies of the ANNNI model.

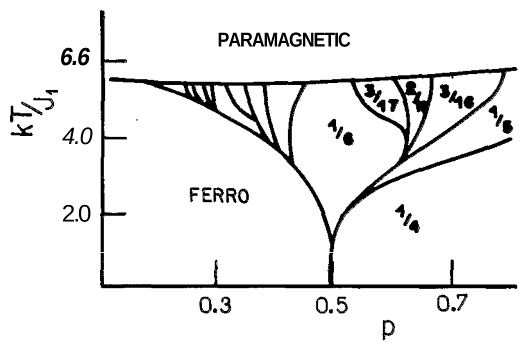

Fig.1 - Sketch of the T-p phase diagram of the ANNNI model, for $J_0 = J_1$, in the standard layer-by-layer mean-field approximation[3].The paramagnetic lines are obtained analytically. We indicate the regions corresponding to the main commensurate phases.

In a previous publication[7], a variational principle, based on a free trial hamiltonian, has been used to derived the layer-by-layer mean-field results for the global T-p-H phase diagram of the ANNNI model. In the present paper, we use the same variational procedure, but introduce a more complex trial hamiltonian, which includes some interactions between pairs of nearest-neighbor spins belonging to the same xy planes. We analyze the stability of the modulated phases under these extra spin fluctuations and provide some quantitative comparisons with both the high-temperature series results and the Monte Carlo analyses. Our results confirm the stability of the modulated phases and show a quantitative trend towards the Monte Carlo data. After the completion of this work, we learned about two independent attempts to improve the mean-field calculations for the ANNNI model. Pires and collaborators[8] use the same variational scheme, with a trial hamiltonian consisting of a set of non-interacting one-dimensional Ising models along the z direction, including first and second neighbor interactions. In this approximation, which should be excellent for $J_0 << J_1, -J_2$, it is not difficult to obtain expressions for the paramagnetic lines and the location of the Lifshitz point. However, it becomes an extremely cumbersome task to analyze the modulated region. In another work, Taylor and Desjardins[9] perform a numerical calculation based on Kikuchi's cluster-variational method. As we shall see below, their results are in qualitative agreement with our findings.

The layout of this paper is as follows. In section 2 we introduce the approximate formulations and obtain the minimization conditions for the free energy. The T-p phase diagram is studied in section 3. We obtain analytic expressions for the paramagnetic lines, the location of the Lifshitz point, and the asymptotic form of the first-order ferromagnetic-modulated boundary near the Lifshitz point. Some numerical calculations, according to the scheme of von Boehm and Bak, as well as comparison with Monte Carlo data, are reported in section 4. Finally, some concluding remarks are presented in section 5.

2. APPROXIMATE FORMULATIONS

The approximate solutions presented in this paper are based on Bogoliubov's inequality

$$G \leqslant G_0 + \langle H-H_0\rangle_0 \equiv \Phi \quad , \tag{2.1}$$

where G is the fsee energy associated with the ANNNI model defined by eq. (1.1), G_0 is the free energy associated with a trial hamiltonian H_0, and the expectation value, $\langle H-H_0\rangle_0$, is taken with respect to H_0. In the standard layer-by-layer mean-field approximation[3,7], H_0 involves terms of the type

$$h_1(z) = -\eta_z^{(1)} S_{x,y,z} \quad . \tag{2.2}$$

According to the work of Ferreira *et al*[10], in the so-called pair approximation, we should also include terms of the type

$$h_2(z) = -J_0 S_{x,y,z} S_{x+1,y,z} - \eta_z^{(2)} \left(S_{x,y,z} + S_{x+1,y,z}\right) , \tag{2.3a}$$

and

$$h_2'(z) = -J_0 S_{x,y,z} S_{x,y+1,z} - \eta_z^{(2)} \left(S_{x,y,z} + S_{x,y+1,z}\right) , \tag{2.3b}$$

where the interactions are restricted to nearest neighbors belonging to the same xy plane. In the so-called square approximation, we should in addition include terms of the type

$$\begin{aligned} h_4(z) = &- J_0 \left[S_{x,y,z} S_{z,y+1,z} + S_{x,y,z} S_{x+1,y,z} \right. \\ &\left. + S_{x+1,y,z} S_{x+1,y+1,z} + S_{x,y+1,z} S_{x+1,y+1,z}\right] \\ &- \eta_z^{(4)} \left[S_{x,y,z} + S_{x,y+1,z} + S_{x+1,y,z} + S_{x+1,y+1,z}\right] . \end{aligned} \tag{2.4}$$

(A) The pair approximation

In the pair approximation the trial hamiltonian is given by

$$H_0 = \sum_z \left[\sum_{xy} h_1(z) + \sum_{xy}{}' h_2(z) + \sum_{xy}{}'' h_2'(z)\right] , \tag{2.5}$$

where the first xy sum is over free spins, while the second and third sums are over isolated pairs of interacting nearest-neigbor spins along the x and y directions respectively. If we call n_2 the number of isolated pairs of interacting spins in each plane, the right hand side of inequality (2.1) is a function of the parameters $\eta_z^{(1)}$, $\eta_z^{(2)}$, and n_2.

It is easy to show that

$$G_0 = - kT\, n_1 \sum_z \log\left[2 \cosh \beta\eta_z^{(1)}\right] - kT\, n_2 \sum_z \log\left[2\, e^{\beta J_0} \cosh 2\beta\eta_z^{(2)} + 2\, e^{-\beta J_0}\right] , \tag{2.6}$$

where $\beta = 1/(kT)$, $n_1 = N^2-2n$, and N^2 is the number of sites in each xy plane. In zero field, if we call m_z the uniform magnetization per spin in the z plane, we have

$$\langle H-H_0\rangle_0 = -\left[2N^2 - n_2\right] J_0 \sum_z m_z^2 - \frac{1}{2} N^2 J_1 \sum_z m_z\left[m_{z-1} + m_{z+1}\right] - \frac{1}{2} N^2 J_2 \sum_z m_z\left[m_{z-2} + m_{z+2}\right] + \sum_z\left[N^2\eta_z^{(1)} + 2n_2\left(\eta_z^{(2)} - \eta_z^{(1)}\right)\right] m_z , \tag{2.7}$$

where

$$m_z = \tanh \beta\eta_z^{(1)} = \frac{\sinh 2\beta\eta_z^{(2)}}{\cosh 2\beta\eta_z^{(2)} + e^{-2\beta J_0}} . \tag{2.8}$$

It should be remarked that this equation, which comes from the assumption that m_z is uniform throughout the xy planes, gives a relation between the parameters $\eta_z^{(1)}$ and $\eta_z^{(2)}$.

The minimiration of Φ with respect to $\eta_z^{(1)}$, with n_2 fixed, yields the relation

$$\frac{2n_2}{N^2}\, \eta_z^{(2)} + \frac{n_1}{N^2}\, \eta_z^{(1)} - J_1\left(m_{z-1} + m_{z+1}\right) - J_2\left(m_{z-2} + m_{z+2}\right) - 2J_0\left(2 - \frac{n_2}{N^2}\right) m_z = 0 , \tag{2.9}$$

where $\eta_z^{(2)}$ and m_z are given by eq.(2.8). Ferreira *et al*[10] use the first terms of the exact high temperature expansion of the free energy to choose the number n_2 of isolated pairs in the trial hamiltonian. According to this criterion, we have $n_2 = 2N^2$, which considerably simplifies eq. (2.9). Then, we may write the minimization conditions as a set of coupled equations for m_z, given by

$$2\beta\eta_z^{(2)} = \frac{3}{4}\log\frac{1+m_z}{1-m} \quad 2 \quad \ldots_{z-1} + m_{z+1}\Big) + J_2\Big(m_{z-2} + m_{z+2}\Big)\Big]\Big], \tag{2.10}$$

where $\eta_z^{(2)}$ comes from

$$m_z = \frac{\sinh 2\beta\eta_z^{(2)}}{\cosh 2\beta\eta_z^{(2)} + e^{-2\beta J_0}} . \tag{2.11}$$

This set of equations admits, in general, more than one solution In this case, the physically relevant solution is the one which gives the minimum value of Φ, which is the approximate Gibbs free energy of the model.

(B) The square approximation

In the square approximation the trial hamiltonian includes a term of the type $\sum_z \sum_{x,y} h_4(z)$, where the xy sum is over n_4 isolated squares of interacting pairs of spins. It is straightfsrward to use the same procedures of the preceding paragraphs to obtain an expression for Φ. In particular, with the choice $n_2 = -2N^2$ and $n_4 = N^2$, which comes from a comparison with the first few terms of an exact high temperature expansion of the free energy, we can write the minimization conditions as the following set of coupled equations for m_z

$$\beta\eta_z^{(4)} = \frac{1}{2}\log\left[e^{-2\beta J_0} m_z + \sqrt{1 + m_z^2\left(e^{-4\beta J_0} - 1\right)}\right]\Big/(1-m_z)$$

$$- \frac{1}{8}\log\frac{1+m_z}{1-m_z} \quad \frac{\beta}{4}\left[J_1(m_{z-1} + m_{z+1}) + J_2(m_{z-2} + m_{z+2})\right],$$

(2.12)

where $\eta_z^{(1)}$ comes from

$$m_z = \frac{e^{4\beta J_0} \sinh 4\beta\eta_z^{(4)} + 2 \sinh 2\beta\eta_z^{(4)}}{e^{4\beta J_0} \cosh 4\beta\eta_z^{(4)} + 4 \cosh 2\beta\eta_z^{(4)} + e^{-4\beta J_0} + 2} \; . \qquad (2.1'3)$$

3. ANALYTIC RESULTS FOR THE T-p PHASE DIAGRAM

In the pair approximation, the transition between the disordered $(m_z=0)$ and the ordered $(m_z\neq 0)$ phases can be determined from an asymptotic analysis of eq. (2.10). For small m_z we have

$$\frac{2}{\beta}\left(1 + e^{-2\beta J_0}\right)m_z - \frac{3}{\beta} m_z \approx J_1(m_{z-1} + m_{z+1}) + J_2(m_{z-2} + m_{z+2}) \; . \qquad (3.1)$$

If we introduce the Fourier components of m_z, according to

$$m_z = \sum_q m_q \, e^{iqz} \; , \qquad (3.2)$$

where the sum is over the first Brillouin zone $(-\pi < q < \pi)$, eq. (3.1) yields

$$m_q \approx \frac{\beta}{(2e^{-2\beta J_0} - 1)} J(q) m_q \; , \qquad (3.3)$$

where

$$J(q) = 2J_1 \cos q + 2J_2 \cos 2q \; . \qquad (3.4)$$

At high temperatures, $m_q=0$ for all q. As we decrease the temperature, however, there will be a solution $m_q \neq 0$ for

$$kT_c\left[2\exp\left(-\frac{2J_0}{kT_c}\right) - 1\right] = \max_q J(q) \equiv J(q_c) \; . \qquad (3.5)$$

From this equation, we see that the modulated phase just below the transition will be characterized by a wave number q_c such that

$$\cos q_c = -\frac{\text{[illegible]}}{4J_2} = \frac{1}{4p} \; , \qquad (3.6)$$

whereas $q_c \equiv 0$ in the ferromagnetic phase. For $p < \frac{1}{4}$, the system undergoes a paramagnetic-ferromagnetic transition, given by the temperature $T_0(p)$, such that

$$\frac{kT_0}{J_1}\left[2\,\exp\left(-\frac{2J_0}{kT_0}\right)-1\right] = \frac{J(0)}{J_1} = \frac{3}{2} - 2\Delta p\ , \tag{3.7}$$

where $J(0) = 2J_1 + 2J_2$, and $\Delta p = p - 144$. For $p > \frac{1}{4}$, the system undergoes a pararnagnetic-modulated transition, given by the temperature $T_\lambda(p)$, such that

$$\frac{kT_\lambda}{J_1}\left[2\,\exp\left(-\frac{2J_0}{kT_\lambda}\right)-1\right] = \frac{1}{J_1}\left[-2J_2 - \frac{J_1^2}{4J_2}\right] =$$

$$= \frac{kT_0}{J_1}\left[2\,\exp\left(-\frac{2J_0}{kT_0}\right)-1\right] + 16\Delta p^2 + O(\Delta p^3)\ . \tag{3.8}$$

From eqs. (3.7) and (3.8) it is easy to write the expansions

$$\frac{\Delta T_0}{T_L} = -\frac{1}{a}\,\Delta p - \frac{b}{a^3}\,(\Delta p)^2 + \ldots\ , \tag{3.9}$$

and

$$\frac{\Delta T_\lambda}{T_L} = -\frac{1}{a}\,\Delta p + \frac{1}{a}\left(8 - \frac{b}{a^2}\right)\Delta p^2 + \ldots\ , \tag{3.10}$$

where $\Delta T_0 = T_0 - T_L$, $\Delta T_\lambda = T_\lambda - T_0$, $a = (2J_0/J_1)\exp(-2J_0/kT_L)$, $b = (2J_0/kT_L)a$, and T_L is given by the equation

$$\frac{kT_L}{J_1}\left[\exp\left(-\frac{2J_0}{kT_L}\right)-1\right] = \frac{3}{2}\ . \tag{3.11}$$

It is then clear that the critical lines $T_0(p)$ and $T_\lambda(p)$ meet smoothly at the Lifshitz point (T_L, p_L) with $p_L = \frac{1}{4}$. Since a, b, and $8a^2 - b$, are all positive, we see that the slopes of $T_0(p)$ and $T_\lambda(p)$ have opposite signs at the Lifshitz point. The Lifshitz point is then an inflection point, in agreement with experimental findings forthernagnetic compound MnP[11]. This is a peculiar result which could not have been obtained from the more standard layer-by-layer mean-field calculation.

The analysis of the nature of the ferrornagnetic-rnodulated transition, as well as the establishment of an asymptotic expression for the transition temperature, $T_1(p)$, close to the Lifãhitz point, require the consideration of higher harmonic components of eq.(3.3). Along the lines of Yokoi et al^7, let us write the magnetization per spin in the form

$$m_z = M_1 \cos(q_c z + \phi) + M_3 \cos(3q_c z + 3\phi) + M_5 \cos(5q_c z + 5\phi) + \ldots, \tag{3.12}$$

where the coefficients M_1, M_3, M_5 ... are supposed to be real. Inserting eq. (3.12) into (2.10), and comparing the coefficients of the same harmonics, we obtain the following asymptotic expressions close to the critical line $T_\lambda(p)$

$$M_1 \approx \pm 2 \left\{ 1 - \frac{T\left[2\exp\left(-\frac{2J_0}{kT}\right) - 1\right]}{T_\lambda\left[2\exp\left(-\frac{2J_0}{kT}\right) - 1\right]} \right\}^{\frac{1}{2}} C(T_\lambda), \tag{3.13}$$

with

$$C(T) = \left[\frac{2\exp\left(-\frac{2J_0}{kT}\right) - 1}{3\exp\left(-\frac{2J_0}{kT}\right) - \exp\left(-\frac{6J_0}{kT}\right) - 1} \right]^{\frac{1}{2}}, \tag{3.14}$$

and $M_3 \approx C_3 M_1^3$, $M_5 \approx C_5 M_1^5$, and so on, where C_3, C_5 ..., are structural coefficients. In general, the amplitude of the nth harmonic component, where n is an odd integer, approaches T_λ as $(T_\lambda - T)^{n/2}$. These results indicate that, close to T_λ, the higher harmonic components contribute as perturbations and the modulated phases are fairly well represented by a sinusoidal layer magnetization with wave vector q_c. For incommensurate wave vectors the phase ϕ is arbitrary. For comrnensurate wave vectors, however, the expansion (3.10) is finite, and ϕ is chosen in order to minimize the free energy. As discussed by Yokoi $et\ al^7$, this distinction is not relevant for calculating asymptotic expressions near the Lifshitz point.

In the context of the pair approximation, let us write an expansion for Φ, in zero field, in terms of m_z. Using the Fourier representation (3.12) we have

$$N^{-3}\Phi = f_0 + \frac{1}{4}\left[-\frac{1}{\beta}\left(2\, e^{-2\beta J_0} - 1\right) + J(q_c)\right]M_1^2 + \frac{1}{4}\left[-\frac{1}{\beta}\left(2\, e^{-2\beta J_0} - 1\right) + J(3q_c)\right]M_3^2 - \frac{3}{32}\left[1 - \left(e^{-2\beta J_0} - 1\right)^2\left(2 + e^{-2\beta J_0}\right)\right]\left[M_1^4 + \frac{4}{3}M_1^3 M_3\right] + \ldots, \quad (3.15)$$

where

$$f_0 = kT \log 2 - 2kT \log\left[2 \cosh \beta J_0\right] . \quad (3.16)$$

Taking into account the temperature dependence of the amplitudes M_1, M_3, ..., we have the following asymptotic expression for the approximate free energy of the modulated phase, near the Lifshitz point,

$$N^{-3}\Phi^{(m)} = f_0 - \frac{kT_L}{2}\left(2\, e^{-2\beta_L J_0} - 1\right)\left[1 - \frac{T\left(e^{-2\beta J_0} - 1\right)}{T_\lambda\left(e^{-2\beta_\lambda J_0} - 1\right)}\right]^2 C^2(T_L) \quad (3.17)$$

In the ferromagnetic phase, $m_z = m$ for all z. It is then easy to obtain

$$m \approx \pm\sqrt{3}\left[1 - \frac{T\left(2e^{-2\beta J_0} - 1\right)}{T_0\left(2e^{-2\beta_0 J_0} - 1\right)}\right]^{\frac{1}{2}} C(T_L) , \quad (3.18)$$

and

$$N^{-3}\Phi^{(f)} = f_0 - \frac{3}{4}kT_L\left(2e^{-2\beta_L J_0} - 1\right)\left[1 - \frac{T\left(2e^{-2\beta J_0} - 1\right)}{T_0\left(2e^{-2\beta J_0} - 1\right)}\right]^2 C^2(T_L). \quad (3.19)$$

Comparing eqs. (3.17) and (3.19) we find that $T_1(p)$ is asymptotically given by

$$\frac{kT_1}{J_1}\left[2 \exp\left(-\frac{2J_0}{kT_1}\right) - 1\right] = \frac{kT_0}{J_1}\left[2 \exp\left(-\frac{2J_0}{kT_0}\right) - 1\right] - (2 + \sqrt{6})16\Delta p^2 + O(\Delta p^3), \quad (3.20)$$

which indicates that T_0, T_λ, and T_1, meet tangentially at the Lifshitz point. Also, we have the same factor $(2+\sqrt{6})16$ which had already appeared in the standard layer-by-layer mean-field calculation. From eqs. (3.17) and (3.19) we can show that the entropy per spin undergoes a jump, of order $(\Delta p)^2$, across the border $T_1(p)$. This confirms the first-order nature of the ferromagnetic-modulated transition.

Similar calculations, with identical results from the qualitative point of view, can be performed within the framework of the square approximation. As the equations become more awkward, we omit all the intermediate steps and only give the expressions for $T_0(p)$, $T_\lambda(p)$, and T_1(p). Then we have

$$\frac{kT_0}{J_1} A\left(\frac{2J_0}{kT_0}\right) = \frac{3}{2} - 2\Delta p \,, \qquad (3.21)$$

$$\frac{kT_\lambda}{J_1} A\left(\frac{2J_0}{kT_\lambda}\right) = \frac{kT_0}{J_1} A\left(\frac{2J_0}{kT_0}\right) + 16\,\Delta p^2 + O(\Delta p^3)\,, \qquad (3.22)$$

and

$$\frac{kT_1}{J_1} A\left(\frac{2J_0}{kT_1}\right) = \frac{kT_0}{J_1} A\left(\frac{2J_0}{kT_0}\right) - (2+\sqrt{6})16\,\Delta p^2 + O(\Delta p^3)\,, \qquad (3.23)$$

where

$$A(x) = \frac{e^{-2x} - 4\cosh x + 5}{1 + e^{2x}} \,. \qquad (3.24)$$

From these equations we see that $T_0(p)$, $T_1(p)$ and $T_\lambda(p)$ meet smoothly at the Lifshitz point, $p_L = 1/4$, and T_L given by

$$\frac{kT_L}{J_1} A\left(\frac{2J_0}{kT_L}\right) = \frac{3}{2} \,. \qquad (3.25)$$

Also, it is straightforward to show that the $T_1(p)$ border remains first-order.

In fig.2 we depict graphs of T_1, T_0, and T_λ, for $J_0 = J_1$, in various approximations. Also, we show the high temperature series results for the critical lines. As expected, the pair approximation gives

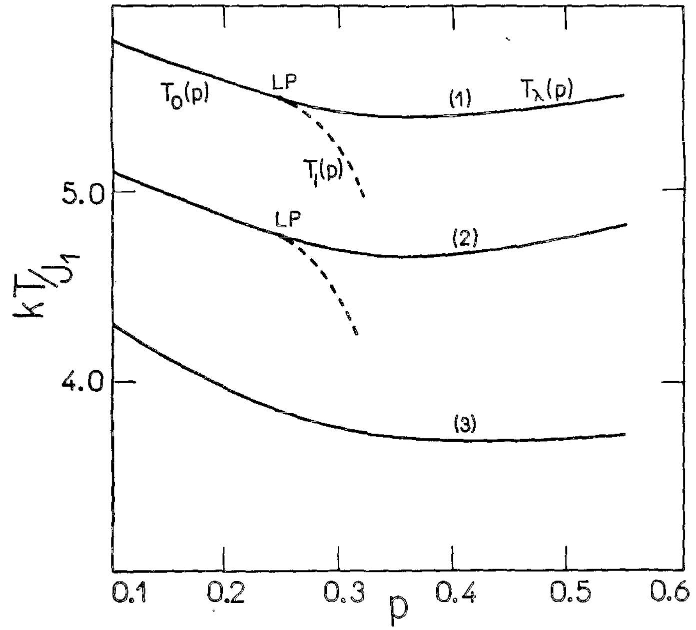

Fig.2 - The high-temperature boundaries of the T-p phase diagram. Phe full lines are the second-order paramagnetic borders, $T_0(p)$, $T_\lambda(p)$. The dashed line, $T_1(p)$, is the asymptotic form of the first-order boundary near the Lifshitz point (LP). (1) Standard layer-by-layer mean-field approximation. (2) Pair approximation. (3) Results from the analysis of the high-temperature series expansions.

lower critical temperatures than the standard layer-by-layer mean-field predictions. The square approximation, however, does not represent a significant improvement. Again, it should be remarked that, in the pair and square approxímations, the Lifshitz point is an inflection point of the paramagnetic border, in agreement with the experimental results for *MnP*.

4. NUMERICAL RESULTS IN THE MODULATED REGION

In the preceding section we have obtained analytic expressions for the layer magnetization per spin m_z in the immediate vicinity of the critical lines. In this asymptotic region, the modulated phase can be well represented by a sinusoidal wave with a wave number q_c depending on the parameter p. As the temperature is decreased, however, higher harmonic components become important, and it is practically impossible to perform analytic calculations. Previous numerical mean-field calculations[3,7] have shown that there are transitions to a sequence of modulated phases, characterized by well-defined values of a principal wave number. At T=0 and $p > 1/2$, the ground state is ferromagnetic, with the wave number $q=0$. However, for $p > 1/2$, the ground state is the antiphase (2,2), given by a sequence of two layers of spins pointing up followed by two layers of spins down, with a wave number $q/2\pi = 1/4$. For $p > 1/4$, it is thus clear that the wave number presents a nontrivial variation with temperature.

The numerical calculations have been performed for $J_0 = J_1$, according to the procedures of von Boehm and Bak[3], and Yokoi *et al.*[7]. In the pair approximation, let us suppose that the solutions of the set of equations (2.10) have a periodicity of L lattice spacings. Under this assumption, the infinite system of equations (2.10) reduces to a system of L non-linear coupled equations, which can be solved self-consistently. As initial conditions we may use sinusoidal structures with different periodicities. Then, for given T and p, we obtain periodic solutions with periodicity L up to 20 lattices spacings, and wave numbers of the form $q/2\pi = K/L$, where $0 \leqslant K \leqslant L \leqslant 20$. At fixed T and p, each solution corresponds to a well defined value of the free energy. Of course, the physically relevant solution is chosen to be the one which minimizes the free energy. It should be remarked that those results are limited to the main commensurate phases, and it is to be understood that in between them there may exist other commensurate or incommensurate phases.

Some results of our numerical calculations are presented in figs. 3 and 4. As in the standard layer-by-layer mean-field approximation, at low temperatures just a few iterations are enough to produce high precision solutions of the set of equations. As the temperature increases, however, the convergence becomes slower, and it is practically impossible to obtain numerical results in the vicinities of the critical lines. Due to the available Monte Carlo data, we looked in detail at the behavior of the wave number for p = 0.6 (see fig. 5). The

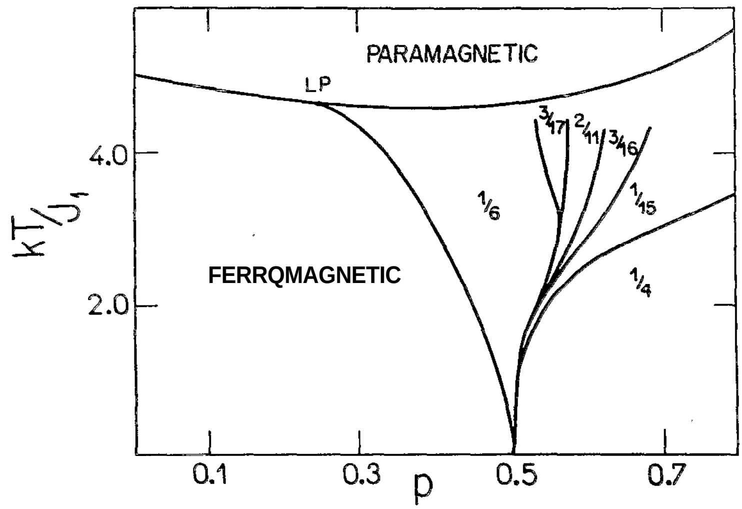

Fig.3 - The main commensurate phases according to the layer-by-layer mean-field calculations in the pair approximation. Also, we show the paramagnetic borders and the first-order paramagnetic-modulated transition line.

results of the palr approximation are qualitatively close to the Monte Carlo findings. Both the Monte Carlo calculations and the palr approximation indicate the same modulated phases and show, unlike the standard layer-by-layer mean-field results, a wave number which decreases monotsnically with temperature. The inclusion of fluctuations in the xy planes affects the regions of stability of the modulated phases butdoes confirm the predictions of both standard mean-field and Monte Carlo calculations.

In fig. 3 we draw the main commensurate phases in the palr approximation. This phase diagram should be compared with the results of von Boehm and Bak (fig.1). Comparing figs. 1 and 3 we see that the transition lines are depressed, and some commensurate-commensurate borders are shifted to smaller values of p. These effects are seen, for example, in the case of the modulated phase $q/2\pi$ = 2/11 (see fig. 4). The results shown in fig. 3 are also in good overall agreement withthecalculations of Taylor and Desjardins[9].

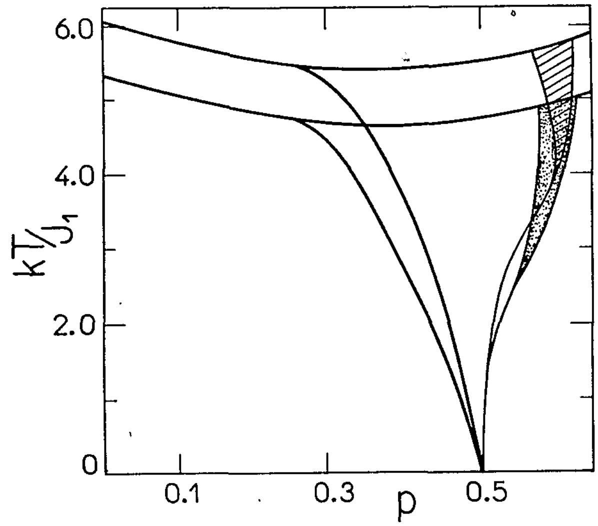

Fig.4 - The T-p phase diagram of the ANNNI model, with special emphasis on the boundaries of the 2/11 phase. The upper curves correspond to the standard mean-field calculation (the 2/11 phase occupies the hatched region). The lower curves correspond to the layer-by-layer mean-field calculation in the pair approximation (in this case, the 2/11 phase occupies the dotted region).

5. CONCLUSIONS

The general features of the phase diagram of the ANNNI model are not changed by the inclusion of some spin interactions in the trial hamiltonian of the layer-by-layer mean-field calculations. As usual, the paramagnetic lines are depressed, in agreement with the analyses based on the high-temperature series expansions. The paramagnetic-modulated and the paramagnetic-ferromagnetic critical lines still meet smoothly, at the Lifshitz point, with the first-order ferromagnetic-modulated transition line. The more refined mean-field calculations show that the Lifshitz point, as in the experiments on the magnetic compound *MnP*, is an inflection point of the paramagnetic border. Numerical calculations

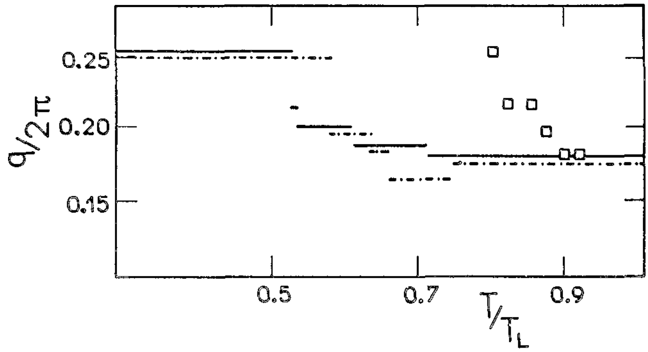

Fig.5 - The wave number versus temperatuse for $p = 0.6$ (see fig. 3). The dot-dashed line corresponds to the standard mean-field calculations. The full line corresponds to the layer-by-layer mean-field calculations in the pair approximation (the square approximation gives almost identical results). The squares correspond to the results from the Monte Carlo data[6].

show that the main commensurate phases are stable under the introduction of the spin fluctuations. For $p = 0.6$, the simple pair approximation yields a wave number which decreases monotonically with temperature, in agreement with results Prom a Monte Carlo analysis. This agreement is slightly improved by using the much more complicated square approximation. In the future we hope to increase the precision of our numerical calculations to test the occurrence of the new structure combination branching processes proposed by Duxbury and Selke[12].

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Resumo

Utilizamos um procedimento variacional,com a inclusão de flutuações de spin, para ir além dos cálculos usuais de camada por camada em campo médio para o diagrama de fases T-p do modelo ANNNI. A região de altas temperaturas é estudada analiticamente. As linhas de transição se encontram suavemente no ponto de Lifshitz, que é um ponto de inflexão da fronteira paramagnética de segunda ordem. A baixas temperaturas, nossos resultados numéricos confirmam a estabilidade das principais fases comensuráveis e mostram uma tendência quantitativa em direção aos resultados obtidos pelo método de Monte Carlo.