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The Classical Ground State of the Axial Next Nearest Neighbour Ising (ANNNI) Model in External Magnetic Fields

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ABSTRACT

We obtain the classical critical antiferromagnetic---paramagnetic and antiphase---paramagnetic phase boundaries of the Axial Next Nearest Neighbour Ising Model in external magnetic fields.

Keywords: classical ground state, ANNNI model, phase boundaries, critical line, magnet ic fields, order parameter.

INTRODUCTION

Frustration as a result of competitive interactions in magnetic models has remained a subject of active research [1,2,3]. The most popular model in which the effects of regular frustration on spin models have been extensively studied is the axial next nearest neighbour Ising (ANNNI) model [4,5]. The ANNNI model is described by a system of Ising spins with nearest neighbour interactions along all the lattice directions (x, y and z) as well as a competing next nearest neighbour interaction in one axial (*e.g.* z) direction.

Recently, there has been an increased interest in transverse Ising models in which the competition is generated by the presence of an external longitudinal field [1,5].

In this paper we will be concerned with an Ising system in which frustration is due to the presence of an external transverse field as well as competitive interactions from next nearest neighbour spins and the influence of an external longitudinal field. Specifically, we will study the one-dimensional ANNNI model in an external transverse magnetic field h_x and a uniform longitudinal field h_z, described by the Hamiltonian

$$H = \sum_i S_i^z S_{i+1}^z + j\sum_i S_i^z S_{i+2}^z - h_x \sum_i S_i^x - h_z \sum_i S_i^z, \quad (1)$$

where j is the next nearest neighbour exchange interaction, S_i are the usual spin-$\frac{1}{2}$ operators and the magnetic fields h_x and h_z are measured in units where the splitting factor and Bohr magneton are unity.

While so far almost exclusively ferromagnetically coupled spins have been discussed in the literature, we will focus this paper on the antiferromagnetic coupling ($j > 0$).

A useful insight into the nature of the phase diagram of the ANNNI model in the presence of two external magnetic fields, described by the Hamiltonian (1) may be gained by first studying its ground state in a classical fashion. This precisely is the aim of this paper. In the next section we will obtain and discuss the possible classical ground state configurations of the ANNNI model in two fields.

RESULTS AND DISCUSSION

In the classical approximation, spins are represented as three-dimensional vectors [1,6,7]. For this purpose let us consider a system of N spins $\frac{1}{2}$. The classical ground state is found from a configuration in which the spin vectors lie in the XZ plane with the N spins pointing respectively at angles φ_1 , φ_2, … and φ_N with respect to the X axis.

2.1 The Classical Ground State of the ANNNI model

In the absence of the fields h_x and h_z , we have the usual ANNNI model, described by the Hamiltonian

$$H_{ANNNI} = \sum S_i^z S_{i+1}^z + j\sum S_i^z S_{i+2}^z . \quad (2)$$

The energy corresponding to the Hamiltonian (2) in the classical description is given by

$$\begin{aligned} E &= \frac{1}{4}\sin\varphi_N \sin\varphi_1 + \frac{j}{4}\sin\varphi_{N-1}\sin\varphi_1 + \frac{j}{4}\sin\varphi_N \sin\varphi_2 \\ &+ \frac{1}{4}\sum_{i=1}^{N-1}\sin\varphi_i \sin\varphi_{i+1} + \frac{j}{4}\sum_{i=1}^{N-2}\sin\varphi_i \sin\varphi_{i+2}, \end{aligned} \quad (3)$$

where we have applied periodic boundary conditions for simplicity. It is also convenient to assume, without loss of generality, that N is a multiple of 4.
The energy E as given in (3) is a minimum if either

1. $\sin\varphi_i \sin\varphi_{i+1} = -1, \quad i = 1,2,\ldots,N-1,$
   and $\sin\varphi_N \sin\varphi_1 = -1$

or

2. $\sin\varphi_i \sin\varphi_{i+2} = -1, \quad i = 1,2,\ldots,N-2$,
   $\sin\varphi_N \sin\varphi_2 = -1$ and $\sin\varphi_{N-1} \sin\varphi_1 = -1$.

Condition 1 implies that

$$\varphi_i = \begin{cases} \pi/2, & i = 1,3,5,\ldots,N-1 \\ -\pi/2, & i = 2,4,6,\ldots,N \end{cases} \tag{4}$$

This corresponds to antiferromagnetic alignment with the ground state energy given by

$$E_{AF}\,/N = -1/4(1-j). \tag{5}$$

The second possibility for a ground state configuration as stated in condition 2 yields the following solution:

$$\begin{aligned} \varphi_{4k+1} = \varphi_{4k+2} &= \pi/2, \quad k = 0,1,2,\ldots, N/4-1 \\ \varphi_{4k-1} = \varphi_{4k} &= -\pi/2, \quad k = 1,2,\ldots, N/4. \end{aligned} \tag{6}$$

This is the period 4 antiphase configuration. The corresponding ground state energy is then given by:

$$E_{<2>}\,/N = -j/4. \tag{7}$$

Comparing equation (5) and equation (7) we see that the classical ground state of the one dimensional ANNNI model (2) is antiferromagnetic for values of the next nearest neighbour exchange interaction $j < \frac{1}{2}$ and the $<2>$ antiphase for $j > \frac{1}{2}$. The ground state is degenerate when $j = \frac{1}{2}$.

2.2 The Classical Ground State of the ANNNI model in external fields

The presence of the transverse field h_x or the longitudinal field h_z or both causes the ground state structure to change. The corresponding classical energy to the full Hamiltonian (1) is then given by

$$E = \frac{1}{4}\sin\varphi_N \sin\varphi_1 + \frac{j}{4}\sin\varphi_{N-1}\sin\varphi_1 + \frac{j}{4}\sin\varphi_N \sin\varphi_2 + \frac{1}{4}\sum_{i=1}^{N-1}\sin\varphi_i \sin\varphi_{i+1} + \frac{j}{4}\sum_{i=1}^{N-2}\sin\varphi_i \sin\varphi_{i+2} - \frac{1}{2}\sum_{i=1}^{N} h_x \cos\varphi_i - \frac{1}{2}\sum_{i=1}^{N} h_z \sin\varphi_i . \tag{8}$$

When $j < \frac{1}{2}$ the ground state structure changes continuously from the ordered antiferromagnetic states described by $\varphi_1 = \varphi_3 = \ldots = \phi_{N-1} = say\ \alpha$ and $\varphi_2 = \varphi_4 = \ldots = \phi_N = say\ \beta$ to the paramagnetic states having constant magnetization. Thus from equation (8) the antiferromagnetic states have energies given by

$$E_{AF}/N = \frac{1}{4}\sin\alpha\sin\beta + \frac{j}{8}\left(\sin^2\alpha + \sin^2\beta\right) - \frac{h_x}{4}\left(\cos\alpha + \cos\beta\right) - \frac{h_z}{4}\left(\sin\alpha + \sin\beta\right). \tag{9}$$

The order parameter, staggered magnetization $M_z^{\pm}$, defined by

$$M_z^{\pm} = \frac{1}{2}\left(\sin\alpha - \sin\beta\right) = \sin\left(\frac{\alpha-\beta}{2}\right)\cos\left(\frac{\alpha+\beta}{2}\right), \tag{10}$$

exists everywhere in the antiferromagnetic region and vanishes on the transition line from the antiferromagnetic phase to the paramagnetic phase. Thus, for a given next nearest neighbour exchange interaction $j < \frac{1}{2}$, the transition line is the set of all h_x and h_z for which E_{AF} in equation (9) is a minimum, with the additional requirement that the order parameter vanishes, *i.e.* that $\alpha = \beta$ in equation (10). Minimizing E_{AF} and taking limit $\alpha \to \beta$ in the resulting critical equations, we find that the antiferro--para phase transition occurs on the line:

$$h_x = (1-j)\cos^3\alpha$$
$$h_z = \sin\alpha\left(1 + \cos^2\alpha + j\sin^2\alpha\right). \tag{11}$$

For $j > \frac{1}{2}$ there is a continuous phase transition from the ordered $< 2 >$ antiphase states described by $\varphi_{4k+1} = \varphi_{4k+2} = say\ \alpha$ for $k = 0,1,2,\ldots,N/4-1$ and $\varphi_{4k-1} = \varphi_{4k} = say\ \beta$ for $k = 1,2,\ldots,N/4$ to the paramagnetic states. Thus from equation (8) the $< 2 >$ antiphase states have energies given by

$$E_{<2>}/N = \frac{1}{4}(\sin\alpha + \sin\beta)^2 + \frac{j}{4}\sin\alpha\sin\beta - \frac{h_x}{4}(\cos\alpha + \cos\beta)$$
$$-\frac{h_z}{4}(\sin\alpha + \sin\beta). \quad (12)$$

The order parameter,

$$M_z^{++--} = \sin\left(\frac{\alpha-\beta}{2}\right)\cos\left(\frac{\alpha+\beta}{2}\right), \quad (13)$$

remains finite everywhere in the $< 2 >$ antiphase region and vanishes on the transition line. Thus, minimizing equation (12) and using the condition $\alpha \to \beta$ in the resulting critical equations, the antiphase--para phase boundary is given by the line

$$h_x = j\cos^3\alpha,$$
$$h_z = \sin\alpha\left(1 + j(1+\cos^2\alpha)\right). \quad (14)$$

The antiferromagnetic to paramagnetic boundary as given by equation (11) is plotted in figure 1 while the antiphase to paramagnetic boundary as given by equation (14) is plotted in figure 2.

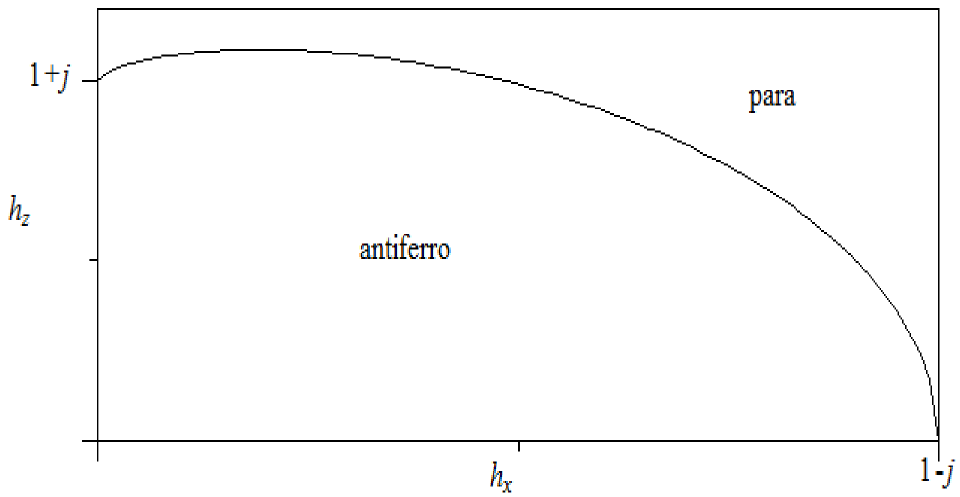

Figure 1: Classical antiferro to paramagnetic phase boundary in the one dimensional ANNNI model in two fields

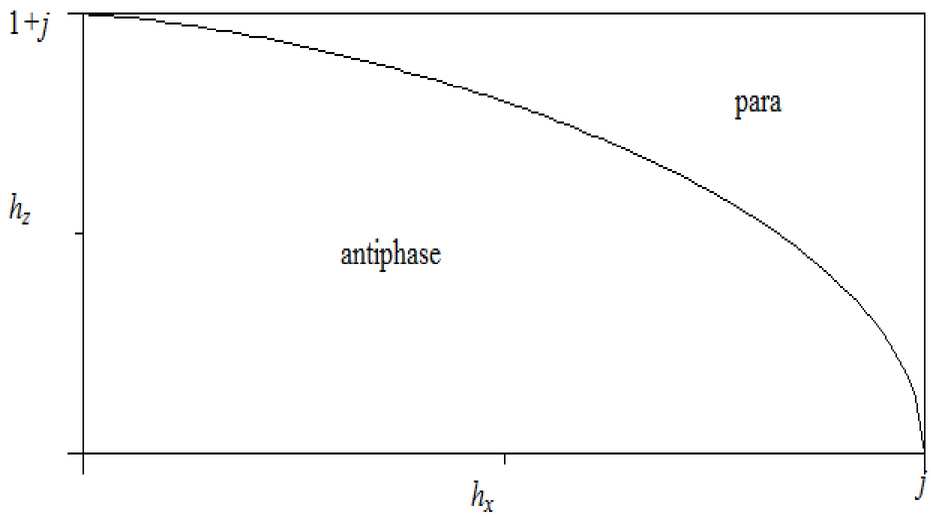

Figure 2: Classical antiphase to paramagnetic phase boundary in the one dimensional ANNNI model in two fields

The two lines equation (11) and equation (14) coincide when $j = \frac{1}{2}$ as expected. We remark also that the special case $j = 0$ (no next nearest neighbour competition) is discussed in [1].

CONCLUSION

We have obtained the classical phase boundaries of the one dimensional ANNNI model in two fields h_x and h_z. We found the critical line separating the antiphase ground state from the paramagnetic phase. We also found the antiferromagnetic--paramagnetic transition line.

The classical results represent of course only very rough approximations of the true behaviour of the ANNNI model in mixed fields. The useful insight gained into the nature of the classical ground states and phase transitions of the model will however serve as a starting point for a more accurate quantum mechanical investigation, as was done for example in [8].

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