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Order disorder transitions in Ising models in transverse fields with second neighbour interactions

Parongama Sen

School of Physical Sciences, Jawaharlal Nehru University, New Delhi 110067, India

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Abstract. The (ferromagnetic) order-disorder transitions in a class of Ising models with second neighbour interaction in transverse fields is studied using the path integral method. Within the limitations of the method, the critical fields at zero temperature are estimated for different systems.

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The effect of quantum fluctuations in classical spin models have been investigated extensively for the last few decades. The simplest of such systems is of course the Ising model in a transverse field [1] which mimics the tunnelling of the proton in hydrogen bonded ferroelectrics. Consequently, other Ising systems, especially those with frustration, in transverse fields, have attracted a lot of interest in the past few years [2]. Examples of such systems are the Ising spin glass system in a transverse field (to model the tunnelling between the localised spin glass states separated by large energy barriers e.g. in $Rb_{1-x}(NH_4)H_2PO_4$, a typical mixed ferroelectric-antiferroelectric hydrogen bonded compound) or the anisotropic next nearest neighbour Ising model [3] (binary alloys like AgMg or polytypes like SiC are systems described by this model) in a transverse field. In the latter, the appearance of novel thermal fluctuation driven phase structures encourages the investigations of the possible transverse field driven transitions.

The path integral formulation of the transverse Ising model [4] has yielded quite accurate values (better than the mean field estimates) for the critical fields for any type of lattice in any dimension above a critical dimension $d = 1$.

This method has also been recently used for treating the frustrated Hopfield model in a transverse field [5]. We apply it to a class of Ising models with second neighbour interaction where the second neighbour interaction can be either ferromagnetic or antiferromagnetic (the latter case will incorporate frustration). Advantage of this method is that one can analytically find out the critical fields in the zero temperature limit. We are primarily interested in the zero temperature limit as we would like to find out the phase transitions driven purely by the transverse field and as also because the systems we will consider have exactly known classical ground states at $T = 0$.

Typically, our Hamiltonian looks like

$$H = -J\sum_{\langle ij\rangle} S_i^z S_j^z - Jx\sum_{\{ik\}} S_i^z S_k^z - \Gamma\Sigma S_i^x \tag{1}$$

where $\langle\ \rangle$ and $\{\ \}$ indicate nearest and next nearest neighbours respectively and $S_i = \pm 1$. When x becomes negative, we have a frustrated system. In all dimensions, the classical ground state for the frustrated case is ferromagnetic for $|x| < 0.5$ and antiphase for $|x| > 0.5$. $|x| = 0.5$ is a highly degenerate point. For the one dimensional frustrated transverse Ising system, several approximation methods have been used to get the phase diagram [2], however, significant results for $|x| > 0.5$ have been obtained from numerical methods only. In higher dimensions, there have been no studies. The method used in the present paper yields results for all dimensions greater than one but is still restricted to $|x| < 0.5$ again.

The equivalent classical Hamiltonian corresponding to (1) is given by the Suzuki Trotter formula:

$$H = -J\left(\sum_t \sum_{\langle ij\rangle} S_i^t S_j^t + x\sum_t \sum_{\{ik\}} S_i^t S_k^t\right)\Big/ P + c/\beta$$
$$+ \ln\coth(\beta\Gamma/P)\sum_i \sum_t S_i^t S_i^{t+1}/2\beta \tag{2}$$

Here t is the Trotter index and P is the Trotter dimension. The constant $c = (1/2)\ln(\cosh(\beta\Gamma/P)\sinh(\beta\Gamma)/P]$

In this Hamiltonian, it can also be interpreted that the spins are effectively P-component vector spins with components $S_j^t = (\pm 1,\ \pm 1,\ \ldots,\ \pm 1)$ where $t = 1, 2, \ldots, P$.

Therefore the partition function of the Hamiltonian in terms of the vector spins becomes

$$Q = \sum_{\{S\}} \exp\left\{\beta J\left(\sum_{\langle ik\rangle} \mathbf{S}_i \cdot \mathbf{S}_k + x\sum_{\{ij\}} \mathbf{S}_i \cdot \mathbf{S}_j\right)\Big/ P + \Sigma \mathbf{S}_i \cdot a\mathbf{S}_i + C\right\} \tag{3}$$

where

$a_{t,t'} = (1/2)\ln\coth(\beta\Gamma/P)\,\delta_{t,t'-1},\ C = NPc.$

The new spin Hamiltonian is now broken up into two parts, a reference part H_0 involving only single site terms and V involving interacting spins such that

$$-\beta H_0 = \sum \boldsymbol{S}_i \cdot a \boldsymbol{S}_i + C \tag{4}$$

and

$$-\beta V = \beta J\left(\sum_{\langle ik\rangle} \boldsymbol{S}_i \cdot \boldsymbol{S}_k + x \sum_{\{ij\}} \boldsymbol{S}_i \cdot \boldsymbol{S}_j\right)\Big/ P. \tag{5}$$

Now we can treat the full Hamiltonian perturbatively such that the free energy F (= lnQ) is given by

$$-\beta F = -\beta F_0 + \sum_n (1/n!)(-\beta)^n C_n(V), \tag{6}$$

with F_0 the free energy corresponding to the unperturbed Hamiltonian Q_0 such that

$$-\beta F_0 = \ln Q_0,$$

with

$$Q_0 = \Sigma \exp(\beta H_0),$$

and the cumulants are given by

$$C_1 = \langle V\rangle_0;\ C_2 = \langle V^2\rangle_0 - \langle V\rangle_0^2 \text{ etc.}$$

The above expression can be regarded as an expansion in successively higher order of fluctuations. With classical systems, the first order term gives the mean field estimate and higher order constitute fluctuation corrections. For the transverse Ising model (with nearest neighbour interaction only) the first order term gives the mean field estimate while the second term grossly improves the result following Kirkwood's prescription of classical spins.

It is convenient to add a generating field at each site $\boldsymbol{h}_j = (h_j/P)(1, 1, \ldots, 1)$, and to impose an order parameter by adding the condition that the average magnetisation vector is

$$\boldsymbol{m} = m(1, 1, \ldots, 1) = \langle S\rangle. \tag{7}$$

The revised reference system partition function is written as

$$Q_0 = \mathrm{Tr}\left(\exp\left(-\beta H_0 + \sum_j \boldsymbol{h}_j \cdot \boldsymbol{S}_j - \boldsymbol{\gamma} \cdot \left[N\boldsymbol{m} - \sum_j \boldsymbol{S}_j\right]\right)\right)$$

where the order parameter condition has been implemented by the Lagrange multiplier vector $\boldsymbol{\gamma} = (\gamma/P)(1, 1, \ldots, 1)$.

The above partition function still corresponds to the partition function of a one dimensional Ising model in a field. In the $P \to \infty$ limit, the free energy of this system is given by

$$-\beta F_0 = \ln Q_0 = -\mathrm{Nm}\gamma + \Sigma \ln\{2\cosh[(\beta\Gamma)^2 + b_j^2]^{1/2} \tag{8}$$

where

$$b_j = (h_j + \gamma)$$

The γ are so chosen that $\partial \ln Q_0/\partial\gamma = 0$ (such that (7) is satisfied). Minimising (8) with respect to m, one gets,

$$m = (\gamma/N)\Sigma \tanh[(\beta\Gamma)^2 + b_j^2)]^{1/2}/[(\beta\Gamma)^2 + b_j^2]^{1/2} \tag{9}$$

We now proceed to calculate the first and second order cumulants. The first cumulant is easily calculated

$$-\beta C_1 = N\beta J(z_1 + z_2 x) m^2/2,$$

where z_1 and z_2 are the coordination number for the first and second neighbour interactions respectively. The free energy is then given by

$$-\beta F/N = -m\gamma + \ln\{2\cosh(\beta\Gamma)^2 + \gamma^2] + \beta J(z_1 + z_2 x) m^2/2.$$

Combining this result with (9), the $m \to 0$ critical line is given by (in the zero longitudinal field)

$$1 = \beta J(z_1 + z_2 x)\tanh(\beta\Gamma)/\beta\Gamma.$$

In the $T \to 0$ limit, it gives the mean field result

$$\Gamma/J = z_1 + z_2 x$$

Next we calculate the effect of fluctuation through the second cumulant term. The second cumulant is given by

$$(2!)^{-1}(-\beta)^2 C_2 = (2!)^{-1}(-\beta)^2(\langle V^2\rangle - \langle V\rangle^2)$$

Following [4] the final expression of C_2 is found to be

$$\begin{aligned}(2!)^{-1}(-\beta)^2 C_2 = (2!)(\beta J/2)^2[&N^2(z_1^2 + z_2^2 x^2 + 2z_1 z_2 x) f_0 \\ &+ N\{z_1(z_1 - 1) + z_2(z_2 - 1)x^2 \\ &+ 2z_1 z_2 x\} f_1 + N\{z_1^2 + z_2^2 x^2] f_2]\end{aligned}$$

where

$$f_0 = -4m^2(\chi - m^2)/N,$$

$$f_1 = 4(m^2\chi - m^4),$$

$$f_2 = 2(\eta - m^4),$$

and

$$\chi = (\gamma/\Lambda)^2 + \{(\beta\Gamma)^2/\Gamma^3\}\tanh\Lambda,$$

$$\eta = (\gamma/\Lambda)^4 + [(\beta\Gamma)^2/2\Gamma^5][4\gamma^2 + (\beta\Gamma)^2]\tanh\Lambda + \{(\beta\Gamma)^4/2\Gamma^4]\operatorname{sech}^2\Lambda;$$

with $\Lambda = [(\beta\Gamma)^2 + \gamma^2]^{1/2}$.

The final expression of the free energy is

$$-\beta F/N = -m\gamma + \ln(2\cosh\Lambda) + (z_1 + z_2 x)\beta J m^2/2 + (\beta J/2)^2(z_1 + z_2 x^2)(\eta - 2m^2\chi + m^4)$$

Minimising F with respect to m, the $T \to 0$ critical line is given by

$$\Gamma/J = [z_1 + z_2 x + \{z_1(z_1 - 5/2) + x^2 z_2(z_2 - 5/2) + 2z_1 z_2 x)\}^{1/2}]/2 \tag{10}$$

Let us now discuss the result (10) for specific systems under consideration.

a. Unfrustrated systems: Although we are more interested in the frustrated systems, an interesting result is obtained for the Ising chain with ferromagnetic interactions for both first and second neighbour (i.e. $x > 0$). The

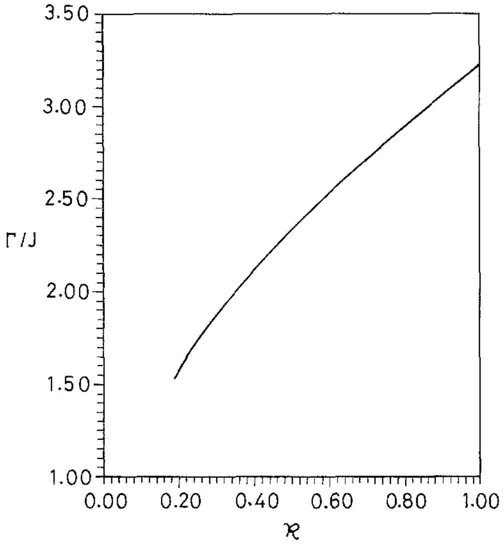

Fig. 1. The critical fields for the unfrustrated extended Ising chain in a transverse field are shown against x

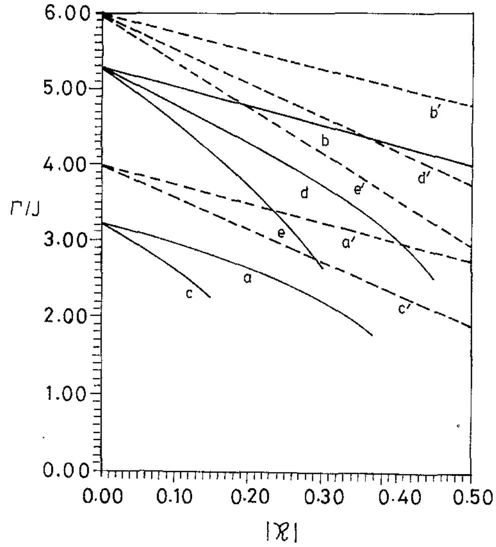

Fig. 2. The critical fields for the ANNNI model in transverse field in two (*a*) and three (*b*) dimensions, BNNNI model in transverse field in two (*c*) and three (*d*) dimensions and the Isotropic next nearest neighbour model in transverse field in three dimensions (*e*) are shown against the frustration parameter ($|x|$) (full curves). The corresponding mean field estimates are shown by the dashed curves

path integral method fails to estimate the zero temperature critical field for one dimension ($z_1 = 2$, $z_2 = 0$). However, with $x > 4 - \sqrt{15}$, one can get estimates of the critical fields even for one dimension. The results are shown in Fig. 1. One might be tempted to extrapolate the result for $x \to 0$, where, the exact result $\Gamma/J = 1$ is obtained for the nearest neighbour transverse Ising chain [6]. Inclusion of a ferromagnetic second neighbour interaction effectively increases the dimension of the system, hence one gets results when x is sufficiently large and no results for small x (where it is still one dimension like) in accordance with the results of [4] where only the first neighbour interaction was considered.

b. Frustrated systems where $x < 0$. These cases will correspond to models like Axial next nearest neighbour Ising (ANNNI), biaxial next nearest neighbour Ising (BNNNI) models etc. The classical ground states here have interesting structures. At a critical value of x (the fully frustrated point), highly degenerate ground states appear above which one gets modulated phases. Hence, we cannot estimate the values of Γ for all values of x as we are only considering $m \to 0$ critical lines. There will be certain values of x where m is already zero at zero field (e.g. the classical modulated ground states like the antiphase with two spins up and two spins down alternately) and therefore cannot be considered here. Also, the $m \to 0$ transitions now indicate transitions from a ferromagnetic phase to either a paramagnetic phase or a modulated phase with $m = 0$. Therefore, the vanishing of the ferromagnetic order appears to be the major result of this method when applied to these systems. We take the example of the following models in one, two (square lattice) and three (cubic lattice) only.

1. The ANNNI model: In all dimensions, we are restricted to $x < 0.5$, as the antiphase with $m = 0$ is the classical ground state beyond this value. In one dimension, again there is no solution. In two dimensions, we find that results are obtained only upto $x < 0.38$. In three dimensions, there is no problem in estimating Γ upto $x < 0.5$.

2. The BNNNI model can be considered in two or three dimensions again with $x < 0.5$.

3. Isotropic next nearest model ($x < 0.5$).

The mean field results as well as those obtained considering first order fluctuations are shown in Fig. 2. The mean field results are largely improved by including fluctuations in the nearest neighbour transverse Ising model, and one believes that even in the frustrated cases, it remains true. Clearly, the ferromagnetically ordered region gets shrunk when one considers fluctuations.

However, when one includes fluctuations it is found that there are some restricting values of x upto which critical fields can be calculated. The restrictions become more important for lower dimensions and higher values of $|x|$ (in case of frustrated systems). Since the approximation is known to be more accurate in higher dimensions, the increasing limitations in the lower dimensions are not surprising. Moreover, we find that this approximation also becomes weaker in the frustrated cases as the frustration parameter is made more effective. On the other hand, in the unfrustrated ($x > 0$) one dimensional version we get estimates of the critical fields beyond a certain value of x. In fact, this approximation tends to effectively increase the spatial dimension in the unfrustrated cases and therefore is able to yield results for one dimension also as already mentioned. The opposite happens in case of the frustrated cases; although here one cannot be sure whether the phase transitions cease to exist at the limiting values of x (beyond which results are not available) or it is simply the failure of the approximation.

One might, perhaps, expect better results when higher order terms are included. In the frustrated cases, a detailed and more accurate phase diagram maybe obtained if one considers spin correlations instead of the magnetisation only, which is beyond the scope of the present method. However, wherever results are obtained (especially for higher dimensions), they are certainly better than mean field estimates.

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