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

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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$_4$)$_x$H$_2$PO$_4$, 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 $d_c$.

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

$$H = - J \sum_{\langle ij \rangle} S_i \cdot S_j - J_x \sum_{\langle ik \rangle} S_i \cdot S_k - J_z S_i \cdot S_j$$  \hspace{1cm} (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:

$$H = - J \left( \sum_{\langle ij \rangle} S_i \cdot S_j + x \sum_{\langle ik \rangle} S_i \cdot S_k \right) \right) \right) / P + c/\beta \right) + \text{lncoth}(\beta \Gamma/P) \sum_{i} S_i \cdot S_i \right) \right) / 2\beta \right)$$  \hspace{1cm} (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 $S_j = (\pm 1, \pm 1, \ldots, \pm 1)$ where $t = 1, 2, \ldots, P$.

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

$$Q = \sum_{\{S\}} \exp \left\{ \beta J \left( \sum_{\langle ij \rangle} S_i \cdot S_j + x \sum_{\langle ik \rangle} S_i \cdot S_k \right) \right) / P + \sum S_i \cdot aS_i + C \right) \right)$$  \hspace{1cm} (3)
where
\[ \alpha_{r'} = (1/2) \ln \cosh(\beta \Gamma / P) \delta_{r'r}, \quad C = N P c. \]

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
\[ -\beta H_0 = \sum \mathbf{S}_i \cdot \mathbf{a} \mathbf{S}_i + C \] (4)
and
\[ -\beta V = \beta J \left( \sum \mathbf{S}_i \cdot \mathbf{S}_k + x \sum \mathbf{S}_i \cdot \mathbf{S}_j \right) / P. \] (5)

Now we can treat the full Hamiltonian perturbatively such that the free energy \( F = \ln Q \) is given by
\[ -\beta F = -\beta F_0 + \sum (1/n!) (-\beta)^n C_i (V), \] (6)
with \( F_0 \) the free energy corresponding to the unperturbed Hamiltonian \( Q_0 \) such that
\[ -\beta F_0 = \sum \ln Q_0, \]
and the cumulants are given by
\[ C_1 = \langle V \rangle_0; \quad C_2 = \langle V^2 \rangle_0 - \langle V \rangle_0^2 \text{ etc.} \]

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 \( h_j = (h_j / P)(1, 1, \ldots, 1) \), and to impose an order parameter by adding the condition that the average magnetisation vector is
\[ \mathbf{m} = m(1, 1, \ldots, 1) = \langle \mathbf{S} \rangle. \] (7)

The revised reference system partition function is written as
\[ Q_0 = \text{Tr} \left( \exp \left( -\beta H_0 + \sum_j h_j \cdot \mathbf{S}_j - \gamma \left[ N m - \sum_j \mathbf{S}_j \right] \right) \right) \]
where the order parameter condition has been implemented by the Lagrange multiplier vector \( \gamma = (\gamma / P)(1, 1, \ldots, 1) \).

The above partition function still corresponds to the partition function of a one dimensional Ising model in a field. In the \( P \rightarrow \infty \) limit, the free energy of this system is given by
\[ -\beta F_0 = \ln Q_0 = -N m \gamma + \Sigma \ln \{ 2 \cosh [(\beta \Gamma)^2 / 2] \}^{1/2} \] (8)

where
\[ b_j = (h_j + \gamma) \]

The \( \gamma \) are so chosen that \( \partial \ln Q_0 / \partial \gamma = 0 \) (such that (7) is satisfied). Minimising (8) with respect to \( m \), one gets,
\[ m = (\gamma / N) \sum \tanh \left( [(\beta \Gamma)^2 / 2]^{1/2} \right). \] (9)

We now proceed to calculate the first and second order cumulants. The first cumulant is easily calculated
\[ -\beta C_1 = N \beta J \langle z_1 + z_2 x \rangle m^2 / 2, \]
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
\[ -\beta F_1 / N = - m \gamma + \ln \{ 2 \cosh (\beta \Gamma)^2 + \gamma^2 \} + \beta J (z_1 + z_2 x) m^2 / 2. \]

Combining this result with (9), the \( m \rightarrow 0 \) 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 \( T \rightarrow 0 \) 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
\[ (2!)^{-1} (\beta J)^2 C_2 = (2!)^{-1} (\beta J)^2 \left( \langle V^2 \rangle - \langle V \rangle^2 \right) \]
Following [4] the final expression of \( C_2 \) is found to be
\[ (2!)^{-1} (\beta J)^2 C_2 = (2!) (\beta J / 2)^2 \left[ N^2 (z_1^2 + z_2^2 x^2 + 2 z_1 z_2 x) f_0 \right. \]
\[ + N \left( \langle z_1 (z_1 - 1) + z_1 (z_2 - 1) x^2 \right. \]
\[ + 2 z_1 z_2 x \rangle f_1 \rangle \]
\[ \left. + N \left( \langle z_1^2 + z_2^2 x^2 \rangle f_2 \right) \right. \]
where
\[ f_0 = -4 m^2 (\chi - m^2) / N, \]
\[ f_1 = 4 (m^2 \chi - m^2), \]
\[ f_2 = 2 (\eta - m^4), \]
and
\[ \chi = (\gamma / A)^2 + \{(\beta \Gamma)^2 / 3\} \tanh A, \]
\[ \eta = (\gamma / A)^4 + \{(\beta \Gamma)^2 / 2 \} \left[ 4 \gamma^2 + (\beta \Gamma)^2 \right] \tanh A \]
\[ + \{(\beta \Gamma)^4 / 2 \} \text{sech}^2 A, \]
with \( A = [(\beta \Gamma)^2 + \gamma^2]^{1/2} \).

The final expression of the free energy is
\[ -\beta F_1 / N = - m \gamma + \ln (2 \cosh \Lambda) + (z_1 + z_2 x) \beta J m^2 / 2 \]
\[ + \{(\beta J / 2)^2 (z_1 + z_2 x^2) (\eta - 2 m^2 \chi + m^4) \}
Minimising \( F \) with respect to \( m \), the \( T \rightarrow 0 \) critical line is given by
\[ \Gamma / J = \left[ z_1 + z_2 x + \{ z_1 (z_1 - 5 / 2) + x^2 z_2 (z_2 - 5 / 2) \right. \]
\[ + 2 z_1 z_2 x \rangle]^{1 / 2} / 2 \] (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