Quantum Phase Transitions in the Ising model in spatially modulated field

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The phase transitions in the transverse field Ising model in a competing spatially modulated (periodic and oscillatory) longitudinal field are studied numerically. There is a multiphase point in absence of the transverse field where the degeneracy for a longitudinal field of wavelength λ is $(\frac{1+\sqrt{5}}{2})^{2N/\lambda}$ for a system with N spins, an exact result obtained from the known result for $\lambda = 2$. The phase transitions in the Γ (transverse field) versus h_0 (amplitude of the longitudinal field) phase diagram are obtained from the vanishing of the mass gap Δ. We find that for all the phase transition points obtained in this way, Δ shows finite size scaling behaviour signifying a continuous phase transition everywhere. The values of the critical exponents show that the model belongs to the universality class of the two dimensional Ising model. The longitudinal field is found to have the same scaling behaviour as that of the transverse field, which seems to be a unique feature for the competing field. The phase boundaries for two different wavelengths of the modulated field are obtained. Close to the multiphase point at h_c, the phase boundary behaves as $(h_c - h_0)^b$, where b is also λ dependent.

PACS numbers: 64.60.Cn, 64.60.Fr, 42.50.Lc

I. INTRODUCTION

Competitive interactions in magnetic models can generate frustration leading to the existence of a large number of degenerate states [1]. For example, in the ANNNI (axial next nearest neigbour Ising) model [1–3], the presence of a second neighbour antiferromagnetic interaction induces a competition. In absence of any fluctuation, a large number of degenerate states exist at a so called multiphase point. In spin glasses [4], interactions are random, and the mixture of ferromagnetic and antiferromagnetic interactions result in frustration and huge degeneracy.

Phase transitions, both classical and quantum, in many of these systems are well studied [1–6]. While the short range Ising like models do not have any finite temperature phase transition in one dimension, the phase diagram in higher dimensions often shows very rich structures. The quantum phase transitions are present even in one dimension. It is interesting to observe that the zeroth order thermal fluctuation in two dimensions and correspondingly zeroth order quantum fluctuations in one dimension can destroy all order at the fully frustrated multiphase point [3,5] in ANNNI-like models.

The Ising models in transverse field form a special class of quantum systems and to the best of our knowledge, have different features in comparison to quantum spin models in which the quantum effect comes through the cooperative interaction.

In this paper, we will discuss a quantum Ising model with competition, where the competition is generated by the presence of an external longitudinal field which is spatially periodic. We choose the periodicity of the field to be commensurate with the lattice periodicity. The field is also oscillatory so that the net field on the entire system sums out to zero. Classically, the ferromagnetic Ising system will not undergo any phase transition in a uniform field. On the other hand, spatially modulated fields can play important roles in critical phenomena. Classical systems in periodic potential (Frenkel-Kontorova model), for example, show very interesting features leading to novel concepts like the devil's staircase [7].

Some interesting and relevant features of the model in the classical limit are discussed in section II. The phase transitions in the ferromagnetic model in the modulated field in one dimension at zero temperature driven by quantum fluctuations generated by the transverse field are described in section III. The results are discussed and concluding remarks are made in section IV.

II. THE MODEL: CLASSICAL GROUND STATE AND DEGENERACY

The Hamiltonian for the system with N spins is given by

$$H_q = -J\sum_{i=1}^{N} S_i^z S_{i+1}^z - \sum_{i=1}^{N} h_i S_i^z. - \Gamma \sum_{i=1}^{N} S_i^x. \qquad (1)$$

The form of the longitudinal periodic field h_i is like this: $h_i = h_0$ at $i = (n\lambda + 1)$ to $(2n+1)\lambda/2$ ($n = 0, 1, ..., N/\lambda - 1$) and $-h_0$ elsewhere. The wavelength of the field is denoted by λ. Γ is the strength of the transverse field.

Note that the modulated field can be chosen to be of various forms, for simplicity we will choose a square wave form. While the ferromagnetic interaction tries to align the spins parallely, the periodic field will try to modulate the system spatially. We will consider periodic boundary condition.

We will first discuss some known results in the context of our model in the classical limit (i.e., $\Gamma = 0$). The classical Hamiltonian is

$$H_{cl} = -J \sum_{i=1}^{N} S_i^z S_{i+1}^z - \sum_{i=1}^{N} h_i S_i^z. \qquad (2)$$

Let us first take the case $\lambda = 2$: the field is positive on odd sites and negative on even. Now one can simply use a transformation $S_{2i}^z \to -S_{2i}^z$. This effectively makes the Hamiltonian

$$H_{cl} = J \sum_{i=1}^{N} S_i^z S_{i+1}^z - h_0 \sum_{i=1}^{N} S_i^z, \qquad (3)$$

i.e, an antiferromagnetic system in a uniform field [8,9] which is solved exactly by transfer matrix method.

Again, if we consider the ANNNI chain, the Hamiltonian is:

$$H_{ANNNI} = -J_1 \sum_{i=1}^{N} S_i^z S_{i+1}^z + J_2 \sum_{i=1}^{N} S_i^z S_{i+2}^z. \qquad (4)$$

The above can be cast to the form of (3) by the transformation $S_i^z S_{i+1}^z \to S_i^z$ [1] with J_1 playing the role of h_0 and J_2 the role of J. Note that J_2 is positive, describing antiferromagnetic interaction by definition. The sign of J_1 is unimportant.

The two models described by equations (3) and (4) are well studied [8,1,3] and they have similar classical ground states: upto $J/h_0 = 0.5$ (or $J_2/J_1 = 0.5$), the system is antiferromagnetic (ferromagnetic for ANNNI when $J_1 > 0$), and paramagnetic (modulated for ANNNI) beyond this value. An infinite number of degenerate states exist at this point. The degeneracy can be calculated exactly [1,8] and is equal to τ^N where $\tau = (1+\sqrt{5})/2$. In the language of the original classical model defined in (2) with $\lambda = 2$, one has ferromagnetic phase upto $h_0/J = 2$ and paramagnetic phase for $h_0/J > 2$.

Even when $\lambda \neq 2$, one can rescale the system by a factor of $\lambda/2$ so that the Hamiltonian is effectively written as in (3). It can easily be checked that the multiphase point is now at $h_c/J = 4/\lambda$ and the degeneracy given by $\tau^{2N/\lambda}$.

It is extremely important to note here that although the antiferromagnetic and ferromagnetic systems have identical critical behaviour, the presence of a field makes things drastically different. Therefore the modulated field in the ferromagnetic system is effectively a uniform field in the mapped antiferromagnetic system. We will specifically take the interaction to be ferromagnetic in order to avoid any ambiguity or confusion.

III. QUANTUM PHASE TRANSITION AND PHASE DIAGRAM AT T=0

There are two limits in which the results are exactly known for the quantum Hamiltonian (1) at zero temperature. The classical limit $\Gamma = 0$ is already discussed. In the limit $h_0 = 0$, the problem is also exactly solved [10]: there is a phase transition at a finite value of the transverse field: $\Gamma_c(0)/J = 1$. This is a quantum critical point and the phase transition is continuous in nature. In a spatially periodic and oscillatory longitudinal field which is competing in nature, the phase transition should occur even at lower values of the transverse field, $\Gamma_c(h_0)$.

Vanishing of the mass gap $\Delta(= E_1 - E_0$ where E_1 and E_0 are the energies of the first excited and the ground state respectively) in the thermodynamic limit is a signature of a continuous phase transition. We obtain the mass gaps for finite chains of length L ($N = L^d = L$, where d the dimensionality is one here).

We employ Lanczos' method to diagonalise the Hamiltonian matrix which is calculated in the basis in which S^z is diagonal. The field being spatially modulated and also commensurate with the lattice periodicity, the system sizes are restricted to specific values for a given wavelength. On the other hand, one requires data for different system sizes for a finite size scaling procedure. Since it is difficult to work with large sizes in a diagonalisation scheme anyway, we have obtained the phase diagrams for $\lambda = 2$ and 4 only. The maximum size taken for both cases is $L = 16$. The result for a very large value of λ can be easily guessed.

We indeed find that Δ vanishes with $1/L$ not only for small values of h_0 but right upto the critical field $h_c = 4J/\lambda$. The critical points $\Gamma_c(h_0)$ can be obtained by extrapolation, and a more accurate estimation is done using finite size scaling of the mass gap, which shows scaling behaviour. We defer a detailed discussion on the scaling of mass gaps and nature of transitions and first summarise the results for the phase diagram.

In Fig. 1, the phase diagrams for $\lambda = 2$ and 4 are shown. We have calculated the ferromagnetic order: $\langle m \rangle = \frac{1}{L}\sum \langle S^z \rangle$ as well as the "staggered magnetisation" defined as $\frac{1}{L}\sum \langle S_i^z h_i \rangle / h_0$. The phase boundary we obtain separates a ferromagnetic phase with nonzero $\langle m \rangle$ and a paramagnetic phase with $\langle m \rangle = 0$. However, since the longitudinal field is always present, the staggered magnetisation is nonzero all over the paramagnetic phase.

It is also observed that as soon as $h_c/J = 4/\lambda$ is reached, the system behaves as if only a field is present and therefore no phase transition is observed here for any non-zero Γ: the mass gap remains finite in the thermodynamic limit almost without any system size dependence. As in some other models with competing interactions, in this model also, the zeroth order quantum fluctuation destroys the order at h_c and lifts the degeneracy.

The entire phase boundary could not be fit to any simple form; we could obtain the behaviour close to the multiphase point quite accurately for both $\lambda = 2$ and $\lambda = 4$. Here the phase boundary appears to be of the form $(4/\lambda - h_0/J)^b$ where $b = 0.77 \pm 0.02$ for $\lambda = 2$ and $b = 0.49 \pm 0.01$ for $\lambda = 4$.

For $\lambda \to \infty$, the critical field $h_c \to 0$, the ferromagnetic phase exists only for $h_0 = 0$, and the phase boundary will coincide with the $h_0 = 0$ axis. The exponent b decreases with λ, ultimately vanishing for $\lambda \to \infty$.

We end this section with a discussion on the scaling behaviour of mass gaps and the nature of phase transitions. In zero longitudinal field, the finite size scaling for the mass gap gives:

$$\Delta \sim L^{-z} f((\Gamma - \Gamma_c) L^{1/\nu}) \tag{5}$$

where z is the dynamic exponent and ν is the correlation length exponent. $z = 1$ and $\nu = 1$ for the one dimensional transverse field Ising model. The latter can be mapped to a two dimensional classical Ising model. f is a universal scaling function.

We find the above finite size scaling form to be valid for non-zero values of h_0 in the sense that when $L\Delta$ is plotted against $(\Gamma - \Gamma_c(h_0))L^{1/\nu}$ the data for different system sizes again collapse for any value of h_0 (see Fig 2). The data collapses are obtained with $z = 1$ and $\nu = 1$ for all h_0, indicating that the model belongs to the universality class of the two dimensional classical Ising model even for non-zero longitudinal modulated fields. As h_0 is increased, the collapse gets limited to a smaller region. The scaling function depends on the value of h_0.

The phase transition points depend on the values of both Γ and h_0. The plots in Fig. 2 are done by keeping h_0 fixed and varying Γ around the critical value. One can study the scaling the other way also: keep Γ fixed and vary h_0. We find that there is a collapse of data for different sizes again, as shown in Fig. 3. The striking feature is that the scaling argument is $(h_0 - h_c(\Gamma))L^{1/\nu}$ with $\nu = 1$. This shows that the competing longitudinal field scales in the same way as does the transverse field. The results for $\lambda = 4$ show the same scaling behaviour as in Figs 2 and 3. We discuss this feature again in section IV.

One may conclude from the above observations that the phase transitions are continuous everywhere (except at $\Gamma = 0$) as the mass gaps vanish continuously and show scaling behaviour as in conventional critical phenomenon.

IV. DISCUSSIONS AND CONCLUSIONS

The Ising model in the presence of a transverse field and a longitudinal field cannot be solved exactly. Recently, most of the studies on transverse Ising models have involved randomness in the transverse field, interactions or longitudinal field. We have considered a very simple model in which there are both quantum effects and frustration, where the frustration comes as a result of the modulated nature of the external field and no randomness is involved.

In absence of the transverse field, the system has a multiphase point. The degeneracy at the multiphase point in the absence of fluctuations is easily calculated for any λ from the known result corresponding to $\lambda = 2$.

We have obtained the phase diagram of the model in the $\Gamma - h_0$ plane at zero temperature using numerical methods. Our results show that a continuous phase transition occurs everywhere except at the multiphase point where $\Gamma_c = 0$ and a first order phase transition is known to exist. The transition at this point is of first order in the sense that the order parameter (magnetisation) discontinuously vanishes at this point. The values of the critical exponent z and ν obtained in this model are identical to those of the transverse Ising model, showing that the periodic longitudinal field is irrelevant. Thus it belongs to the classical two-dimensional Ising universality class.

Our conclusions are based on the scaling behaviour of the mass gap. As in conventional critical phenomena, it shows finite size scaling behaviour close to the critical point. It is to be noted that according to scaling arguments in classical critical phenomena, there are only two relevant fields for magnetic systems, temperature (T) and magnetic field (h), and the correlation length scales as:

$$\xi = L \; g((L^{1/\nu} t, h L^{(\beta+\gamma)/\nu}). \tag{6}$$

The deviation from the critical temperature is denoted by t, β and γ are the critical exponents associated with the order parameter and susceptibility respectively and g is a universal scaling function. Here the field h and the temperature have different scaling dimensions. There is, however, no criticality associated with the uniform ordering field h. In the present model, the two important quantities are the transverse field and the competing longitudinal field. The quantum fluctuations through Γ may be compared to the thermal fluctuations. The roles of Γ and T may be considered to be equivalent; however, the roles of the competing field and ordering field are completely different. That is why a scaling form as in (6) will not be valid here. On the other hand, from the study of the finite size scaling of the mass gaps (section III), it appears that the competing field and the transverse field have the same scaling behaviour. We claim this to be a unique feature of the non-ordering competing field.

Beyond the multiphase point, the field is dominating, and no continuous phase transition can exist here; the mass gap remains finite in the thermodynamic limit. This is in contrast to the competitive models like ANNNI model, where one obtains phase transitions beyond the fully frustrated point as well. This difference is of course due to the different roles played by interaction and field. The correspondence between the Ising model in competing field and the ANNNI model mentioned in section II is valid only in one dimension and in the classical limit.

From the present study, however, existence of other modulated phases, separated by first order lines, cannot be ruled out. Such a possibility is strongest close to the multiphase point. A closer inspection, eg., using perturbation methods could be done from which it may also be possible to verify the behaviour of the phase boundary and get an estimate of b defined in section III.

A few other points need to be mentioned. In the random field transverse model, a tricritical point was obtained [11]. The phase diagram of certain antiferromagnets like $FeCl_2$ in a uniform field also show a tricritical point. In comparison, our model does not have any such point. Rather, the phase boundary to the left of the multiphase point is very similar to that of the ANNNI model in higher dimensions. In the latter also, the next neighbour interaction cannot change the universality class of the Ising model. The mapping to the antiferromagnetic model in the classical limit and subsequent description of the ground state assumes that we are considering hypercubic lattices only, where, in absence of any field at zero temperature, the antiferromagnet will order. This is not true in lattices in which the antiferromagnetic system is geometrically frustrated (e.g., in a triangular lattice); such systems in transverse (and longitudinal) field in two dimensions have been recently studied [12].

We have considered only a square wave form for the modulated field in this discrete model. The features should not be different for a different form, however, there will be quantitative changes. In a continuum model, it may be more convenient to choose a sinusoidal form. More complex spin patterns are obtained in (antiferromagnetic) systems with long range interactions in a field, e.g., the long range antiferromagnet in a uniform field [13] exhibits a complete devil's staircase. It is expected that there will also be very interesting features if the modulation in the field is incommensurate with the lattice periodicity.

The author is grateful to S. Dasgupta, A.Dutta and B. K. Chakrabarti for very useful and enlightening discussions and suggestions. She also thanks I. Bose for comments.

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FIG. 1. The phase boundaries between ferromagnetic and paramegnetic regions are shown for the transverse Ising model in a spatially modulated field for two wavelengths $\lambda = 2$ and 4. Near $h_c(\lambda)/J = 4/(\lambda)$, the boundaries fit to the form $(h_c(\lambda) - h_0)^b$, shown by the continuous curves, where $b = 0.77 \pm 0.02$ and 0.49 ± 0.01 for $\lambda = 2$ and $\lambda = 4$ respectively.

FIG. 2. The scaling plot for the scaled mass gaps $L^z\Delta$ with $(\Gamma - \Gamma_c(h_0))L^{1/\nu}$ for $\lambda = 2$. The four sets correspond to the values of $h_0 = 1.9, 1.8, 1.6$ and 1.0 from top to bottom, each showing the collapse of data points for $L = 8, 10, 12$ and 16 with $z = 1$ and $\nu = 1$.

FIG. 3. The scaling plot for the scaled mass gaps $L^z\Delta$ with $(h_0 - h_c(\Gamma))L^{1/\nu}$ for $\lambda = 2$. The four sets correspond to the values of $\Gamma = 0.25, 0.45, 0.65$ and 0.95 from top to bottom, each showing the collapse of data points for $L = 8, 10, 12$ and 16 with $z = 1$ and $\nu = 1$.

Fig 1: Phase diagram

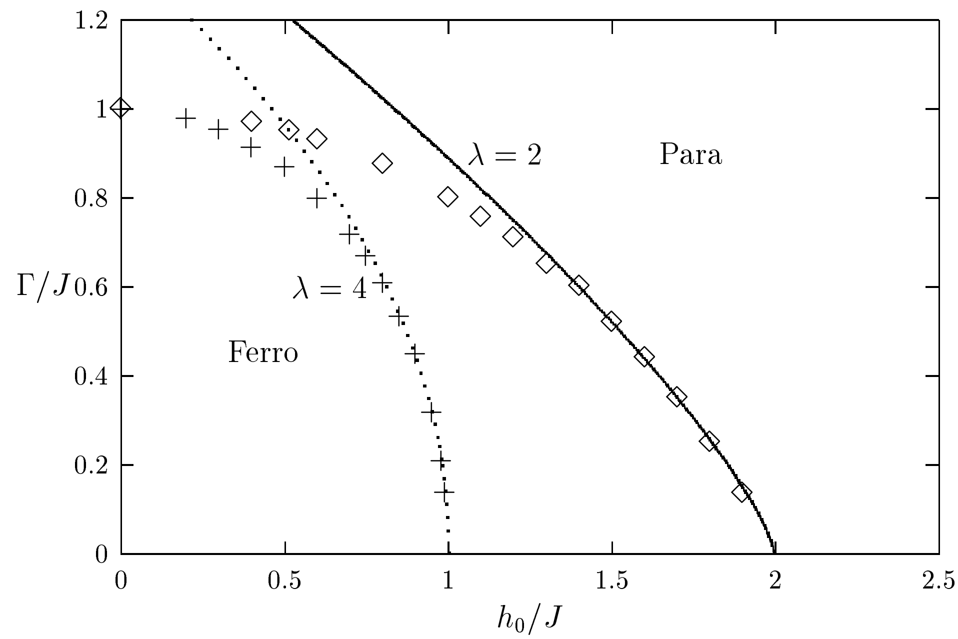

Fig2: Scaling with $\Gamma - \Gamma_c$

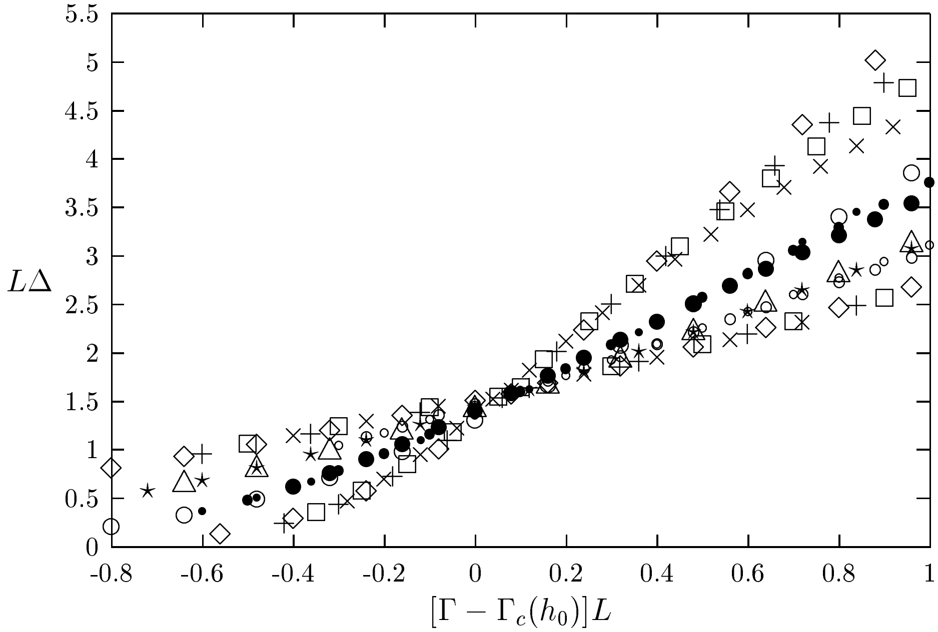

Fig3: scaling with $(h - h_c)$