

Application of the interface approach in quantum Ising models

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We investigate phase transitions in the Ising model and the ANNNI model in transverse field using the interface approach. The exact result of the Ising chain in a transverse field is reproduced. We find that apart from the interfacial energy, there are two other response functions which show simple scaling behavior. For the ANNNI model in a transverse field, the phase diagram can be fully studied in the region where a ferromagnetic to paramagnetic phase transition occurs. The other region can be studied partially; the boundary where the antiphase vanishes can be estimated. [S0163-1829(97)12817-X]

I. INTRODUCTION

Phase transitions in Ising spin systems driven entirely by quantum fluctuations have been getting a lot of attention recently.¹ The simplest of such systems is the Ising model in a transverse field which can be exactly solved in one dimension. Quantum fluctuations in Ising systems with more complicated interactions which, for example, incorporate frustration and or disorder, give rise to novel and intriguing features. Recently, the experimental realization of some cases like the spin glass system in a transverse or tunneling field, have added to the interest in such systems.¹

We apply the method of interfaces² in the Ising model and the anisotropic next-nearest-neighbor Ising (ANNNI) model³ in a transverse field at zero temperature to study the quantum fluctuation driven transitions. In the process, we also explore the scope of the so-called twist method^{2,4} which we have shown to have additional features apart from the ones already known.

Recently, it has been shown in a variety of spin systems how the interfaces caused by twisting a system are closely linked to the phase transition. Apart from the application of the twist method to several classical models like Ising spins systems, the Potts model, and spin glasses,² very recently it has been used for quantum ground state problems also.⁴ In this method, the interface free energy is generated by the excess free energy between systems with and without a twist. In general, twisting the system may be done by changing the boundary condition in one direction. The idea is that long range order produces stiffness. The interface free energy, which is the response to the stress generated by the twist provides direct information on the stiffness of the ordered state. For classical systems, i.e., in a thermally driven phase transition, this method analyzes size (L) and temperature (T, T_c the critical temperature) dependence of the stiffness free energy (which is the increment of free energy due to the change ϕ in boundary conditions) defined by

$$\Delta F = F_\phi - F_0, \quad (1)$$

where F_ϕ and F_0 are the free energy with and without twist, respectively. ΔF has the simple scaling form^{5,2}

$$\Delta F = A[(T - T_c)L^{1/\nu}]L^{\alpha(T)}, \quad (2)$$

where the stiffness exponent α is a constant for $T < T_c$, equal to zero for $T = T_c$ and negative for $T > T_c$. Hence the critical point can be obtained from $\alpha(T_c) = 0$. In Ising spin systems with nearest-neighbor interactions, $\alpha = d - 1$, where d is the dimension of the system. For frustrated systems, α may be nonintegral.²

On the other hand, in phase transitions driven by quantum fluctuations at zero temperature, one needs to consider only the ground state energy (which is equivalent to the free energy) and here the interfacial free energy is expected to have a different stiffness exponent.

We have applied the twist method in two quantum systems: first to reproduce the exact result of the Ising chain in a transverse field⁶ and then to the ANNNI model in a transverse field.¹ In the latter, there are additional frustration effects which have to be taken under consideration. Our results show that apart from the interfacial free energy, there are at least two other response functions which carry information of the phase transition and follow simple scaling laws. In Sec. II, we describe the method used to study the quantum Ising models as well as the results. The results are discussed in Sec. III.

II. METHOD AND RESULTS

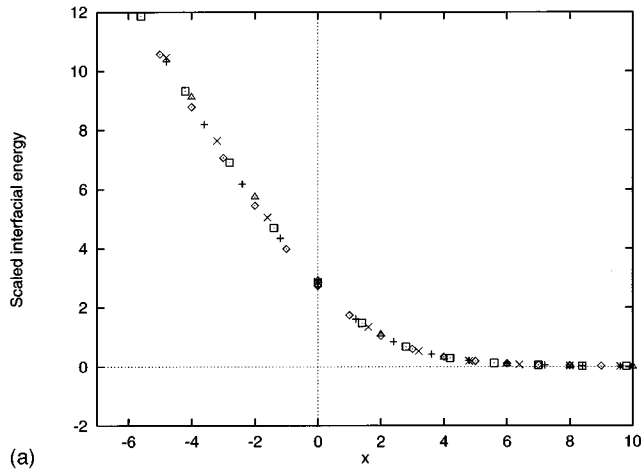
The stiffness exponent for the quantum model at zero temperature is defined in the same way as in Eq. (2), the role of temperature now being assumed by the transverse field such that

$$\Delta E = E_0 - E_\phi = g[(\Gamma - \Gamma_c)L^{1/\nu}]L^{\phi(\Gamma)}. \quad (3)$$

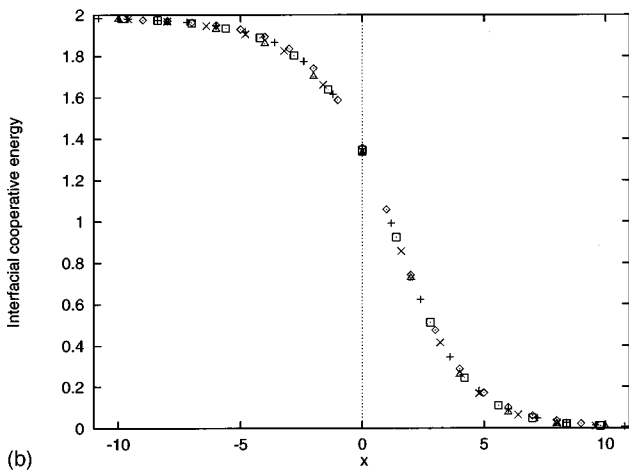
The Ising chain in a transverse field is described by the Hamiltonian

$$H = -J \sum_{i=1}^L S_i^z S_{i+1}^z - \Gamma \sum_{i=1}^L S_i^x \quad (4)$$

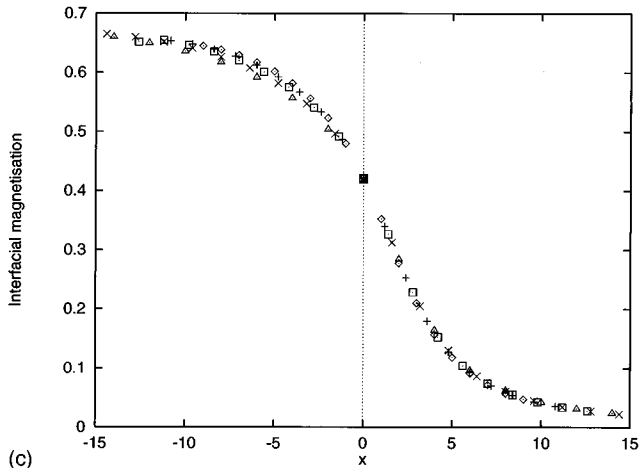
and the ferromagnetic to paramagnetic phase transition occurs at $\Gamma/J = 1$ for $S^z = \pm 1$. We take the basis states to be diagonal in the representation of S^z . The twist is applied in the following way:² in one case we have fixed spins pointing parallelly in the left and right boundaries which favors the ferromagnetic alignment and is called the favorable boundary condition (FBC), while in the other case we have fixed



(a)



(b)

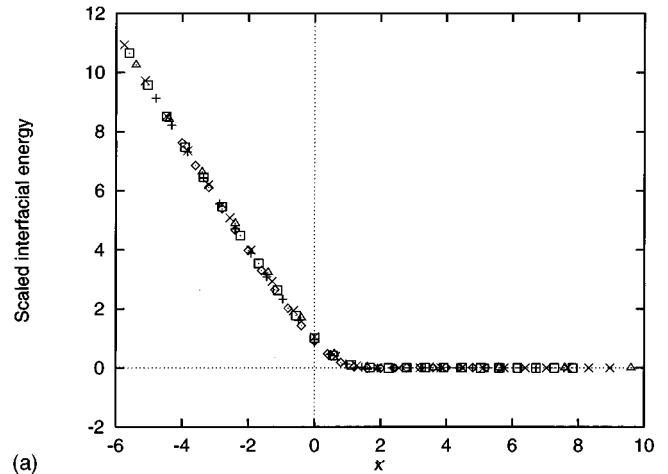


(c)

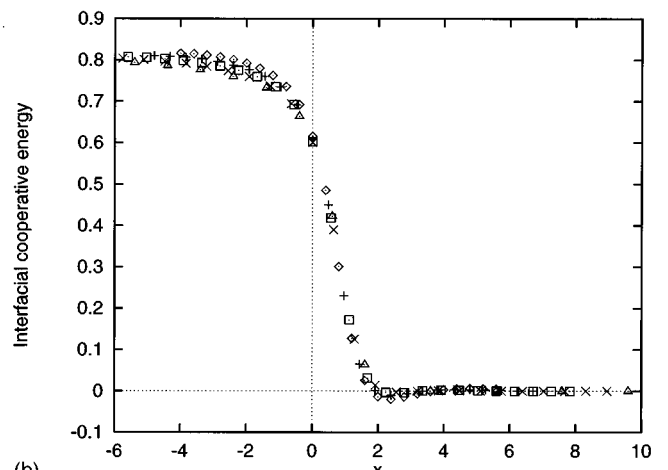
FIG. 1. Plot of (a) ΔEL , (b) ΔE^c and (c) Δm vs $x=(\Gamma-\Gamma_c)L^{1/\nu}$ for system sizes 10 (\diamond), 12 ($+$), 14 (\square), 16 (\times), and 20 (\triangle) for the Ising chain in transverse field with $\Gamma_c = 1$ and $\nu=1$ (E, Γ in units of J).

spins at the boundaries antiparallely oriented (unfavorable boundary condition or UBC). The latter generates an interface and hence the excess energy. The first spin also interacts with the extra spin (fixed) on its left and the last (L th) spin interacts with the extra [$L+1$ th] spin (fixed) on its right.

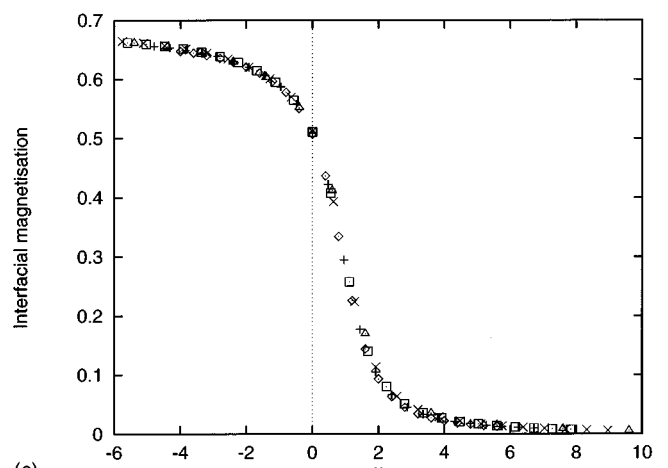
It needs to be clarified here that we have used open boundary conditions with two extra spins pointed either par-



(a)



(b)



(c)

FIG. 2. Plot of (a) ΔEL , (b) ΔE^c and (c) Δm vs $x=(\Gamma-\Gamma_c)L^{1/\nu}$ for system sizes 10 (\diamond), 12 ($+$), 14 (\square), 16 (\times), and 20 (\triangle) for the ANNNI chain in transverse field with $\Gamma_c=0.42$ and $\nu=1$ at $\kappa=0.3$ (E, Γ in units of J).

allely or antiparallely at the edges. This, while generating the interface, will also introduce boundary effects (finite size effects in a numerical study): the two effects are intermingled and difficult to separate. It might be possible to study the interface effect alone by using periodic and antiperiodic boundary conditions,⁷ but that involves more complicated

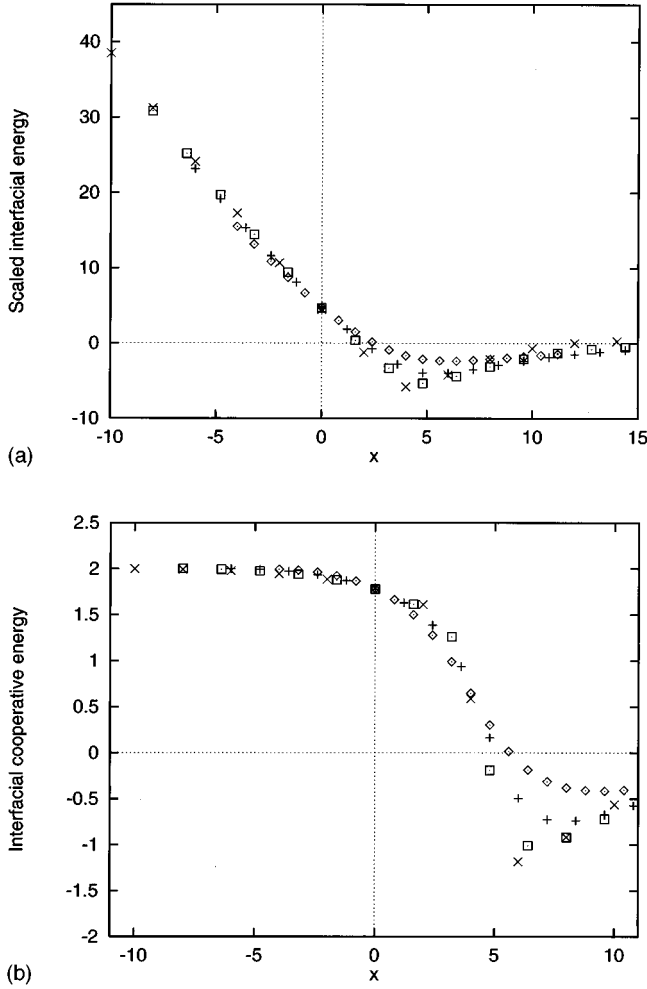


FIG. 3. Plot of (a) ΔEL and (b) ΔE^c vs $x=(\Gamma-\Gamma_c)L^{1/\nu}$ for system sizes 8 (\diamond), 12 (+), 16 (\square), and 20 (\times) for the ANNNI chain in transverse field with $\Gamma_c=0.52$ and $\nu=1$ at $\kappa=1.0$ (E, Γ in units of J).

programming and computer time. Therefore, we have both interface and boundary effects, and when we talk of the interface effect in the rest of the paper, it essentially includes the boundary effect, the latter diminishing with system size.

We proceed to find out the ground state of a system of L spins (excluding the two at the boundary) in a transverse field by using a Lanczos algorithm for both kinds of boundary conditions (FBC and UBC).

Apart from the interfacial energy defined in Eq. (3), we also investigate the behavior of the interfacial cooperative energy and the interfacial magnetization. These two quantities are defined in the following way: let $E^c = \langle \psi | H^c | \psi \rangle$ where H^c is the term(s) in the Hamiltonian involving only the cooperative interaction energy and $|\psi\rangle$ the ground state. For Eq. (4), $H^c = -J \sum_i^L S_i^z S_{i+1}^z$. Then the interfacial cooperative energy is given by

$$\Delta E^c = E^c_0 - E^c_\phi. \quad (5)$$

The interfacial magnetization is similarly defined

$$\Delta m = m_o - m_\phi, \quad (6)$$

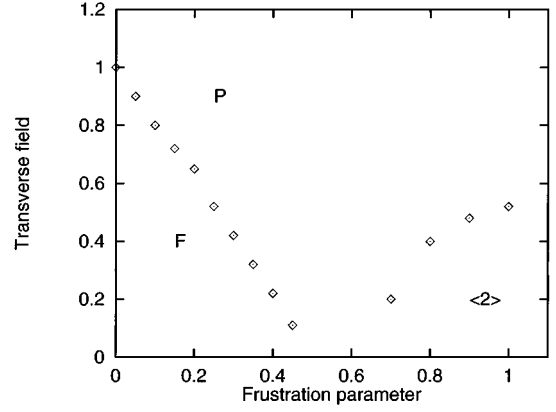


FIG. 4. Partial phase diagram for the ANNNI chain in a transverse field: for the frustration parameter $\kappa < 0.5$ the data points indicate the critical fields for the ferromagnetic (F) to paramagnetic (P) transition, for $\kappa > 0.5$, the data points indicate the disappearance of the antiphase ($\langle 2 \rangle$).

where $m_0(m_\phi)$ is the magnetization in the ground state with (without) twist. We have obtained results for system sizes $L = 6$ to $L = 20$ and studied the behavior of ΔE , ΔE^c , and Δm . All three scale in general as Eq. (3) giving the exact result $\Gamma_c/J=1$ and $\nu=1$ (see Fig. 1). Although the exact critical point is known for Eq. (4), certain other features are available from our study which show novel features of the stiffness exponent for quantum systems. We have discussed these scaling behaviors and commented about them in Sec. III.

We next extend the study to the ANNNI chain in a transverse field. The Hamiltonian is described by

$$H = -J \left(\sum_{i=1}^L S_i^z S_{i+1}^z - \kappa \sum_{i=1}^L S_i^z S_{i+2}^z + \Gamma \sum_{i=1}^L S_i^x \right). \quad (7)$$

Here κ denotes the frustration parameter. The classical ground state without Γ at zero temperature is exactly known: ferromagnetic for $\kappa < 0.5$, antiphase for $\kappa > 0.5$, and highly degenerate phases exist at $\kappa = 0.5$.³ The quantum ANNNI model, which is perhaps the simplest model incorporating both frustration and quantum fluctuation, has been studied extensively (and the corresponding classical model) in the last few years.¹ However, the nature of the ground state and the phase transition is yet to be understood clearly, especially in the region $\kappa > 0.5$. It is believed that a floating phase exists^{1,8} close to the $\kappa = 0.5$ region which has also been found for the classical two-dimensional model in the free fermion approximation.³ All earlier studies indicate that there is a ferromagnetic to paramagnetic transition at $\kappa < 0.5$. Hence, the twist method is easily applicable here in the same manner as in the nearest-neighbor Ising case. In order to impose favorable and unfavorable boundary conditions, we fix two spins on the left and right ends of the chain, and find the ground states. The spins on the boundaries interact with the extra fixed spins as in the Ising case, with open boundary conditions prevailing. For $\kappa < 0.5$, the FBC consists of parallel spins, and for UBC, it is antiparallel just like the nearest-neighbor case. It may be mentioned that one could do without bringing in two fixed spins but we keep this in order that it is consistent with the ground states also at

$\kappa > 0.5$. We have applied here the twist method and found that it gives consistent results in the $\kappa < 0.5$ region where a ferromagnetic to paramagnetic transition occurs. Again we find that ΔE , ΔE^c , and Δm have simple scaling forms and we get the critical field for any $\kappa < 0.5$ in this way. As an example, we have shown the scaling of the three quantities in Fig. 2 for $\kappa = 0.3$.

In the $\kappa > 0.5$ region, we have no clear idea about what kind of a transition is taking place which is clearcut ferromagnetic to paramagnetic in the $\kappa < 0.5$ region. Therefore, all we have attempted to do here is to find out the phase boundary where the antiphase disappears by putting appropriate UBC and FBC for the antiphase. However, there still remains a problem. The frustration effects now become dominant and the ground state is no longer trivially degenerate. This generates not a single interface but maybe more than one. Also, because of the structure of the degenerate ground states due to the presence of both nearest- and next-nearest-neighbor interactions, the so-called unfavorable boundary condition for one particular ground state may become favorable for another degenerate ground state, thus making it difficult to feel the effect of the field due to the twist. For example, if we set the two spins on the left boundary down and the two on the right up, then the state with minimum interaction energy is $|uudd \cdots uudd\rangle$, a member of the set of the four degenerate ground states in the antiphase. Setting all the boundary spins on the left and right down to provide the necessary twist, the new ground state should apparently have a structure $|uu \cdots uu\rangle$, where we do not know how the spins in the interior are oriented. The cooperative energy contribution at the boundary to this state is $2J - 4J\kappa$. However, if we look at another antiphase state which is $|duudd \cdots dduud\rangle$, then the energy contribution at the boundary is $-2J$. Hence it is possible that the latter is lower in energy compared to $|uu \cdots uu\rangle$ especially if $-2J < 2J - 4J\kappa$ or when $\kappa < 1$. Hence, a second antiphase state becomes the ground state when the twist is applied therefore making the present method ineffective. However, with the quantum term also present, we observed from the numerical exercise that this problem disappears for $\kappa \geq 0.7$ where we find out the phase boundary. The interfacial magnetization is of course not meaningful here.

We have estimated the phase boundary where the $\langle 2 \rangle$ phase disappears again from the best scaling plots for ΔE and ΔE_c (the $\kappa = 1.0$ case is shown in Fig. 3). However, the data collapse is not so impressive as in the $\kappa < 0.5$ region. The resulting partial phase diagram is shown in Fig. 4.

III. DISCUSSIONS

We have studied the behavior of essentially three quantities and found that they carry information about the quantum phase transitions in the Ising and ANNNI models in the interface approach. Of these, the behavior of the total interface energy had been known earlier, but the scaling of the interfacial cooperative energy and interfacial magnetization appear to be new results. However, there was earlier evidence that the cooperative energy contribution is significant in a study of quantum spin glasses.^{1,9}

In Ref. 4, it was argued that one should look at the scaling behavior of the quantity $L\Delta E$ which is expected to have a

stiffness exponent = 1 for the transverse Ising chain (the same as that of the $2d$ classical model). However, this is the same as saying ΔE scales as L^0 , and we do not find this behavior (except, of course, at $\Gamma = 0$, but we are interested in the scaling behavior near the critical point). On the other hand, we do find that ΔE^c does have a stiffness exponent 0 (i.e., scales as L^0) while ΔE shows a scaling behavior with a stiffness exponent = -1 [see Figs. 1(a)–1(c) drawn with $\nu = 1$].

Now, in the case of the classical systems, we have the stiffness exponent = $d - 1$. Of course, for $d = 1$, there is no thermal phase transition and therefore the exponent $\alpha = 0$ is never encountered. But, here we do have a phase transition driven by quantum fluctuations and that may be the reason for obtaining an exponent $\alpha = 0$ for the interfacial cooperative energy. The interfacial magnetization also scales with an exponent $\alpha = 0$. The scaling function $g_c(x)$ for the interfacial cooperative energy is also evidently of the following form:

$$g_c(x) = a \quad \text{for } x < 0$$

$$= 0 \quad \text{for } x > 0,$$

where a is a constant depending on κ . It maybe noted that the magnetization depends not only on the number of interfaces but also their positions and it is apparent from the data that as the system size is increased, the interface caused by the twist moves towards the center of the chain. Therefore, the exponent $\alpha = 0$ for the interfacial magnetization is not surprising.

One can say that the nontrivial exponent of -1 obtained for the total interfacial energy is a novel feature of the quantum model. On the other hand, if one looks at the scaling functions in Figs. 1–3, it is obvious that they are different for $L\Delta E$ and ΔE^c . The scaling functions for ΔE^c and Δm are, however, similar. Apparently the scaling function $g(x)$ for $L\Delta E$ has the following form:

$$g(x) \sim -x \quad \text{for } x < 0$$

$$= 0 \quad \text{for } x > 0$$

such that $L\Delta E \sim (\Gamma_c - \Gamma)L$ which is the expected behavior mentioned in Ref. 4.

The scaling behavior of ΔE^c and ΔE are different but the quantities ΔE^c and $L\Delta E$ have the same stiffness exponent. Hence, there is an additional dimension L in the total energy which may be related to the additional dimension which comes into play in quantum models.

That the interface method is quite powerful is again proved. We obtain the exact critical point for the transverse Ising chain and a phase diagram for the transverse ANNNI model consistent with the previous studies. However, we did not venture to investigate the regime $\kappa > 0.5$ in the ANNNI model fully because of the nontrivial nature of the transition to a possible floating phase. The phase boundary where the antiphase disappears is also not obtained for $\kappa < 0.7$ because of the difficulty in imposing conflicting boundary conditions. Since in degenerate systems there can be a number of ways to impose the FBC and the UBC, we tried several combina-

tions but faced the same difficulty. This is because of the very structure of the degenerate ground states as elaborated in Sec. II. It is true that the more interesting phase transitions for $\kappa > 0.5$ could not be obtained here, but we showed that estimating the boundary above which the antiphase vanishes is a nontrivial task itself. In fact, most of the analytical and numerical methods give an incomplete picture for $\kappa > 0.5$.

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¹See, e.g., B. K. Chakrabarti, A. Dutta, and P. Sen, *Quantum Ising Phases and Transitions in Transverse Ising Models*, Lecture Notes in Physics Vol. M41 (Springer-Verlag, Heidelberg, 1996), and the references therein.

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