

Competing multispin interactions

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A generalized $(D + 1)$ -dimensional anisotropic Ising model with a combination of multispin interactions in its D dimensions is introduced. A $(1 + 1)$ -dimensional case ($D = 1$) with competing two- ($\sim J_2$) and four-spin ($\sim J_4$) couplings was analyzed through its one-dimensional Hamiltonian version with the use of the finite-size scaling method. Whereas for small J_4/J_2 the transition is of the usual Ising type, for sufficiently large J_4/J_2 a first-order phase transition occurs. A comparison with other models with competing interactions was made.

I. INTRODUCTION

The competing interactions are known to produce a range of characteristic important effects. The complexity of their phase diagrams is perhaps best illustrated in two-dimensional (2D) lattice-gas models.¹ Such features as intermediate, incommensurable phases,^{2,3} multiphase points with infinitely degenerate ground states with finite entropy,⁴ Lifshitz points,^{5,6} and disorder lines^{7,8} are common to a number of theoretical models.

The competing interactions in these studies usually involve central, pairwise forces of different ranges.⁹ However, it has been long recognized that such forces are merely an approximation.¹⁰

Recently, various multibody interactions are receiving increasing attention¹¹ and are being applied in various fields. A case in point is the magnetic structure of solid ³He which is thought to be caused by four-spin interactions.¹² Multibody forces seem to play important roles in many fields such as surface,^{1,13} plasma,¹⁴ and nuclear physics,¹⁵ and physics of other quantum crystals.¹⁶ Four-spin exchange models have been successfully applied to such magnetic systems as NiS₂ and C₆Eu.¹⁷ Judging from exact results available,¹⁸⁻²¹ the multibody interactions have a profound influence on the critical behavior. The transfer matrix of a $D > 2$ Ising model was shown to be related to a Fermion model with multibody interactions.²² The concepts of frustration,²³ duality,²⁴⁻²⁶ etc., extend naturally to multibody interactions. An explicit introduction of such interactions into the field theory appears to be promising.²⁷

It is then natural to ask whether multibody interactions can be made to compete and, if so, what are the effects on the phase diagrams and the critical behavior. The purpose of this work is to introduce a new Ising-type model with competing multispin interactions. The model is then specified to a 2D version which is analyzed through its Hamiltonian representation in a particular case. This paper is organized as follows. In Sec. II the model along with its Hamiltonian representation is introduced. Various soluble limits are indicated and the duality properties are discussed. In Sec. III the phase diagram and the critical behavior are obtained using the finite-size-scaling

(FSS) method. In Sec. IV the ground-state properties, the ground-state energy and the entropy, are obtained. Section V contains conclusions and discussions.

II. THE MODEL AND ITS HAMILTONIAN REPRESENTATION

A possible extension of a conventional Ising model to include multispin interaction consists in allowing n -spin interactions in D -dimensional (hyper)planes of a regular $(D + 1)$ -dimensional system. These D -dimensional subsystems are then coupled by ordinary nearest-neighbor (NN) couplings. The simplest variant of n -spin interactions is just a product of n -neighboring Ising spins in a given domain. Such anisotropic interaction is defined by the Hamiltonian $[\beta = (k_B T)^{-1}]$

$$\beta H' = - \sum_{n \geq 2} \left[K_n \sum_{R_n(D)} \prod_{i \in R_n(D)} S_i \right] - K_0 \sum_{\langle k,l \rangle} S_k \cdot S_l. \quad (1)$$

In (1), $R_n(D)$ is a compact domain in D dimensions containing n spins, and K_n are appropriate “ n -spin exchange” integrals. In the second term the neighboring spins S_k and S_l are in different neighboring domains, and the interaction is in the additional, $(D + 1)$ th dimension only. The notation of (1) is explained in Fig. 1 for a $(D + 1 = 2)$ -dimensional square Ising model which con-

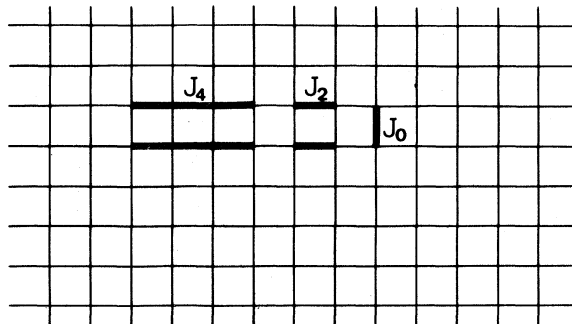


FIG. 1. 2D anisotropic Ising model with two- and four-body interactions.

tains the chains with two- ($\sim J_2$) and four-spin ($\sim J_4$) interactions in one of its dimensions, and the chains are coupled by ordinary NN ($\sim J_0$) interactions. Such a generalized anisotropic Ising model has a quantum Hamiltonian representation in one dimension which can be derived by the transfer-matrix method.²⁸ In the following, for computational reasons (see below), we shall consider the above case of two- and four-spin interactions. Its quantum representation reads

$$H = -J_2 \sum_i S_i^x S_{i+1}^x - J_4 \sum_i S_i^x S_{i+1}^x S_{i+2}^x S_{i+3}^x - h \sum_i S_i^z, \quad (2)$$

where $\vec{S}_i = (S_i^x, S_i^y, S_i^z)$ is the Pauli matrix at the site i [e.g., $S_i^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$] and h is the transverse magnetic field. The coupling constants of the classical and quantum representations are related through the limit $K_2, K_4 \rightarrow 0$ and $K_0 \rightarrow \infty$, if

$$\frac{h}{J_2} = K_2^{-1} \exp(-2K_0), \quad (3a)$$

$$\frac{h}{J_4} = K_4^{-1} \exp(-2K_0) \quad (3b)$$

are kept constant.²⁸

It is in this limit that the transfer matrix of (1) can be shown to commute with (2) and, consequently, the free energy of (1) for finite temperature corresponds to the ground-state energy of (2).²⁸ The natural parameters in which to discuss the ground-state properties of (2) are $g = h/J_2$ [corresponding to the temperature T of (1)] and the ratio $\kappa = J_4/J_2$.

The ground state of (2) can be determined exactly in several limits.

(a) $h=0$ (i.e., $T=0$). In this limit the model becomes classical and its ground state depends on the sign of J_4 . For $J_4=0$, it is a normal Ising doublet, and for $J_2=0$ and $J_4 < 0$, it is an octuplet consisting of repeating patterns of S_i^x ,

$$+----, -+---, \dots, -++++, +-+++, \dots$$

For $0 < |\kappa| \leq 0.5$ the ground state is still doubly degenerate and for $|\kappa| > 0.5$ it is an octuplet. For $|\kappa| = 0.5$ the ground state is highly degenerate.

(b) $J_2 = J_4 = 0$, $h \neq 0$ (i.e., $T \rightarrow \infty$). In this case the ground state is a singlet characterized by $S_i^z = 1$ for all i . The other limits are displaying phase transitions and are less trivial.

(c) $\kappa = 0$, $h \neq 0$. In this case (2) reduces to the Ising model in the transverse field, solved exactly by Pfeuty.²⁹ There exists a phase transition at a self-dual point $(h/J_2)_c = 1$, where the Ising doublet transforms into a singlet. The critical exponents are those of the 2D Ising model (Onsager solution).

(d) $J_2 = 0$, $J_4 \neq 0$ (with arbitrary sign), $h \neq 0$. This situation describes a generalized Ising model with four-spin coupling in a transverse field. Such models were introduced recently²⁴⁻²⁶ and have been analyzed using the molecular-field theory and the FSS methods. There exists a phase transition at a self-dual point $(h/J_4)_c = 1$, where the octuplet transforms into a singlet. This transition is

most probably of (weakly) first order with large, but still finite, correlation length.²⁴

In the following the phase diagram and the critical behavior of (2) away from the above limits will be explored using the FSS methods. From now on we assume $J_4 = -|J_4|$, because for $J_4 > 0$ [see point (a)] no competition between the interactions is possible and the transition disappears.

Some remarks are necessary, in order to justify the particular choice of competing two- and four-body interactions. Firstly, there can be no competition between the interactions of the opposite multiplicity parities; i.e., two- and three-body interactions do not compete— J_3 acting as a longitudinal field and destroying the transition.^{11(a)} Secondly, higher-order interactions can possibly compete, but cannot be reasonably treated by the FSS methods with rather limited sizes of finite blocks. Thus (2) seems to be sufficiently representative for the problem of competition and is still tractable by the existing methods.

III. FSS ANALYSIS

The method of FSS is a powerful tool to analyze the critical properties of interacting systems. The most complete review of theory and applications of FSS has been given recently by Barber.³⁰ The FSS method is particularly useful for complicated interactions, because it does not generate new terms in the Hamiltonian as the other renormalization-group methods do. As applied to (2), the FSS method was used to determine the phase diagram and

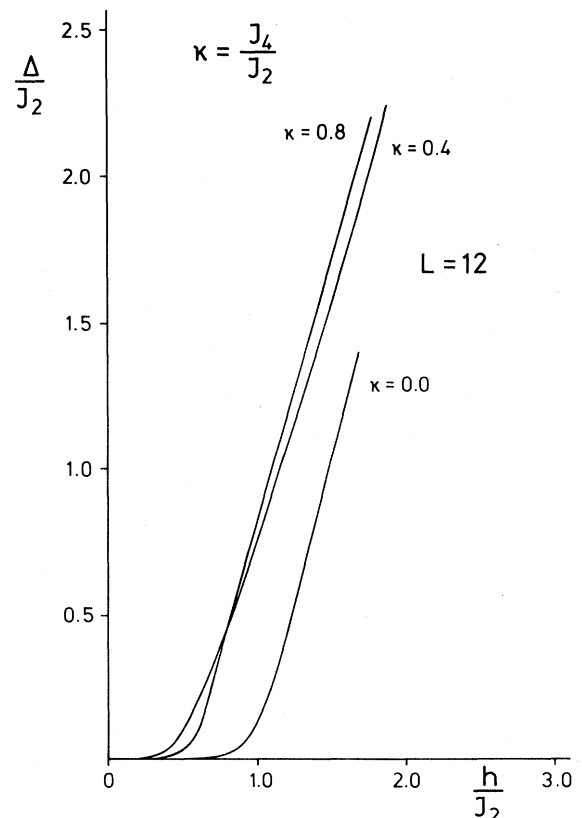


FIG. 2. Energy gap Δ as a function of h/J_2 for few values of κ . $\kappa=0$ corresponds to the Ising model in a transverse field.

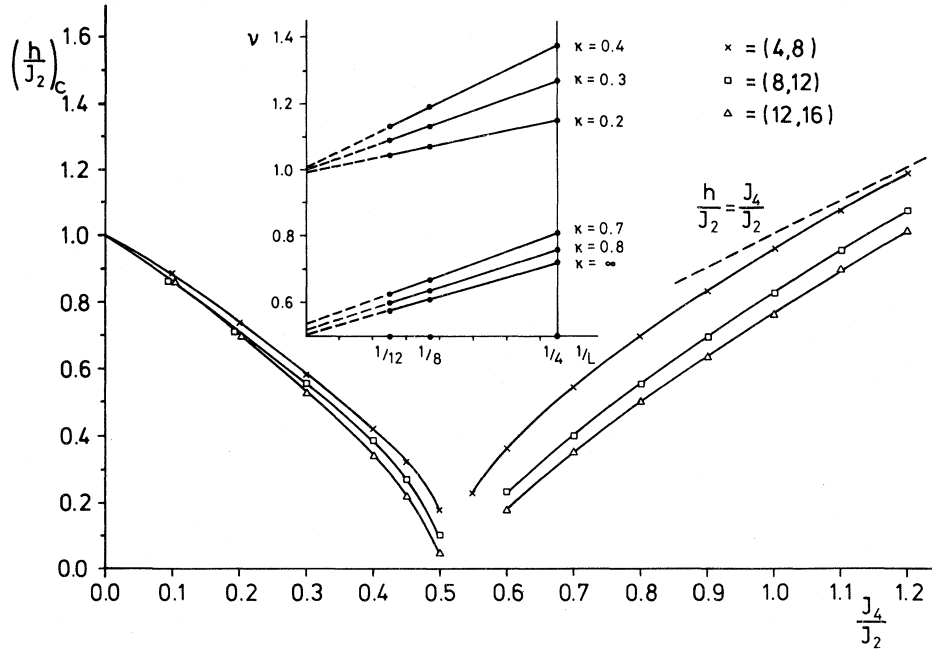


FIG. 3. Critical fields $(h/J_2)_c$ as a function of $J_4/J_2=\kappa$, obtained for different block sizes L ($L \leq 16$). For $\kappa \rightarrow \infty$, the critical field should asymptotically approach the line $h/J_2=J_4/J_2$ (dashed). In the inset the values of the exponent ν for different κ 's are given.

the critical exponents for general values of g and κ . In the space of $g=h/J_2$ and κ there should be a critical line between degenerate and singlet ground states, described by $(h/J_2)_c=F(\kappa)$, with $F(0.5)=0$. At $(h/J_2)_c$ a gap Δ between the singlet ground state and excited states opens,

$$\Delta \sim \left[\frac{h}{J_2} - \left(\frac{h}{J_2} \right)_c \right]^s,$$

where $s=\nu z$, with ν the correlation-length exponent and z the dynamical critical exponent ($z=1$).³¹ For $J_2=0$ or $J_4=0$, (2) is shown to be self-dual^{24,25} with $(h/J_i)_c=1$ ($i=2$ and 4). Consequently, $F(0)=1$ and $\lim_{\kappa \rightarrow \infty} F(\kappa)=\kappa$. The function $F(\kappa)$ and the critical exponent $s=\nu$ have been obtained using the FSS method.

The basic quantity which determines the critical behavior is the energy gap $\Delta \sim \xi^{-1}$ between the ground and first excited states. In order to obtain Δ , the Hamiltonian (2) was diagonalized for finite systems with $L=4, 8, 12$, and 16 spins using the Lanczos scheme. The periodic boundary conditions were assumed. Representative plots of Δ for $L=12$ spins are shown in Fig. 2 as a function of (h/J_2) for various values of κ , and are compared with $\kappa=0$ case (Ising model with transverse field).

The FSS method amounts to calculating the gaps Δ for g and κ for systems of various linear "sizes" L and L' . The basic FSS assertion is that upon the size change $L \rightarrow L'$ the correlation length ξ changes as

$$\xi_L(g, \kappa) = L/L' \xi_{L'}(g', \kappa). \quad (4)$$

This can be reinterpreted as

$$\Delta_{L'}(g', \kappa) = b \Delta_L(g, \kappa), \quad (5)$$

with $b=L/L'$. The fixed points $g^*(L, L'; \kappa)$ of this relation, as obtained from

$$\Delta_{L'}(g^*, \kappa) = b \Delta_L(g^*, \kappa), \quad (6)$$

should tend to the exact values $g_c(\kappa)$ if $L, L' \rightarrow \infty$ with $L/L'=b$ fixed.

The phase diagram obtained from the analysis of fixed points is shown in Fig. 3, and reproduces well the exact features elaborated upon in Sec. II:

- (a) for $\kappa=0$, $(h/J_2)_c=1$,
- (b) $F(\kappa) \rightarrow \kappa$ for $\kappa \rightarrow \infty$, and
- (c) $F(0.5)=0$.

The critical behavior across the phase boundaries of Fig. 3 was obtained by calculating the correlation exponent $\nu_{L, L'}$ for different values of κ from³⁰

$$\left[\frac{L'}{L} \right]^{1+\nu_{L, L'}} = \frac{\dot{\Delta}_{L'}(g^*(L, L'; \kappa))}{\dot{\Delta}_L(g^*(L, L'; \kappa))}, \quad (7)$$

with $\dot{\Delta}_{L'} = d\Delta_{L'}/dg$; see the inset of Fig. 3. For $\kappa \leq \frac{1}{2}$, the $L \rightarrow \infty$ extrapolated value for ν seems to remain equal to 1—its value for the $J_4=0$ case. This suggests that the transition stays Ising-like in character up to $\kappa=0.5$. For $\kappa > 0.6$, the extrapolated values of ν are very close to 0.5. This is very suggestive of first-order phase transition as can be seen from the following arguments. For a quantum system in D dimensions the hyperscaling predicts $(D+z)\nu=2-\alpha$, where z , the dynamical critical exponent, is equal to 1 [exact equivalence to a $(D+1)$ -dimensional classical system³¹]. At the first-order transition point $\alpha=1$,³² and consequently, $\nu=0.5$ for $D=1$. So, for $\kappa > 0.6$ the critical behavior resembles the $J_2=0$ case discussed in Ref. 24, and the transition is presumably of first order.

As seen from Fig. 3 for $0.5 < \kappa < 0.6$, the FSS method fails to give the transition line and, consequently, no

values for exponents could be obtained. It is natural to suppose that there the system enters some sort of modulated phase or sequence of phases and that a transition is XY-like, very much the same as in the 2D case of the axial next-nearest-neighbor Ising (ANNNI) model.⁶ In order to test this hypothesis we have calculated the wave-vector dependence of Δ_L , i.e., $\Delta_L(g, \kappa; q)$ with $q = \pi m/L$ with $m = 0, \pm 1, \dots, \pm(L-1)$. If the ground state of H displayed some q_0 periodicity, then for finite L , in a (g, κ) region in question, a marked minimum

$$\Delta_L(g, \kappa; q_0) = \min_q \Delta_L(g, \kappa, q)$$

should appear, with $\Delta_\infty(g, \kappa; q_0) = 0$, where $q_0 = q_0(g, \kappa)$ and $q_0 \neq \pi/2$.^{5,6} We have calculated, using the same calculational procedure, $\Delta_L(g, \kappa; q)$ for both H and one-dimensional quantum representation of the ANNNI model.³³⁻³⁵ (For the ANNNI model $g = h/J_{NN}$ and $\kappa = J_{NNN}/J_{NN}$.) For the ANNNI model very clear absolute minima of $\Delta_L(g, \kappa; q)$ appeared in the region in which an incommensurate phase was predicted. In contrast, for H no such minima were observed.³⁶ We conclude that, within the FSS method (with available sizes $L \leq 16$), there is no evidence for the existence of an intermediate phase for H for $0.5 < \kappa < 0.6$. However, some kind of crossover effect is taking place with ν (if it exists at all) changing, perhaps continuously with κ between 1 and ~ 0.5 . In the discussion (Sec. V) a heuristic argument against the presence of the incommensurate phase for (2), based on the wall picture will be also given.

IV. GROUND-STATE PROPERTIES

Whereas the correlation properties of quantum models are related to the low-lying parts of the spectrum, their "thermal" properties are determined by the ground-state energy. In this section the ground-state energy $E_0(g, \kappa)$ with its derivatives will be discussed.

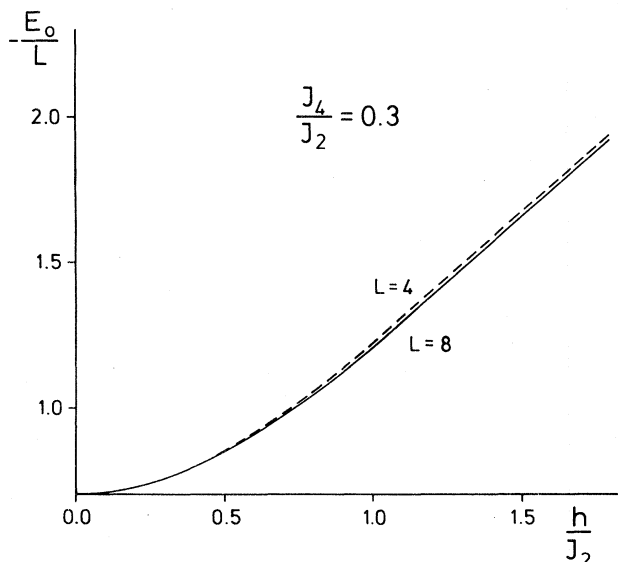


FIG. 4. Ground-state energy per spin as a function of h/J_2 for $\kappa = 0.3$ for blocks of $L = 4$ and 8 spins. The curves for $L = 12$ and 16 are indistinguishable from that of $L = 8$.

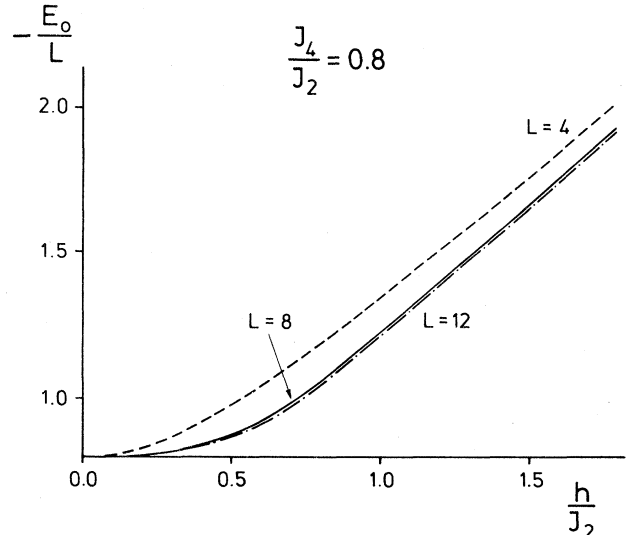


FIG. 5. Ground-state energy per spin as a function of h/J_2 for $\kappa = 0.8$ for blocks of $L = 4, 8$, and 12 spins. The curve for $L = 16$ is practically indistinguishable from that of $L = 12$.

The values of the negative of the ground-state energy per spin $-E_0(g, \kappa)/L$ are shown in Figs. 4 and 5. In Fig. 4, $-E_0(g, \kappa)/L$ is plotted as a function of g for $\kappa = 0.3$. According to Fig. 3 and previous discussion, it corresponds to the Ising-like region. Only $L = 4, 8$ values are presented, since for $L = 12$ and 16 the curves are, on this scale, indistinguishable from that of $L = 8$. In Fig. 5 the same quantity is displayed for $\kappa = 0.8$, i.e., in the region of first-order phase transition. Here, the size dependence is stronger but again the $L = 12$ and 16 curves coalesce. Note that in both cases $E_0(g, \kappa; L)$ is an increasing function of L , showing that the size dependence is not variational in character.

The use of FSS methods for first-order phase transitions is hampered by the fact that, in principle, the correlation length remains finite and the scale invariance is lost at the transition point; this is the basic assumption of FSS methods. A way around this difficulty has been proposed,³² where it has been shown that at the first-order transition points the size dependence of maximas and widths of such diverging (in infinite systems) quantities as the specific heat and the susceptibility is much stronger than at second-order transition points. Analogous criteria based on the renormalization-group formulation of FSS methods were also advanced.^{37,38} They are consistent with the fact that off the true criticality the finite-size free energy approaches exponentially its $L \rightarrow \infty$ limit.³⁰ Although such criteria perform rather well for strongly first-order phase transitions, as in $q \gg 4$ Potts model in 2D,³⁹ it remains to be seen whether they could be useful for weakly first-order cases with very large, but finite correlation length.

The model (2) for $\kappa > 0.5$ appears to be an appropriate candidate because the higher multiplicity couplings ($\sim J_n$ with $n > 4$) almost certainly produce first-order transitions.^{24,25} In view of the above considerations we have explicitly calculated the entropy of the transition for different system sizes. Since the free energy per spin of the

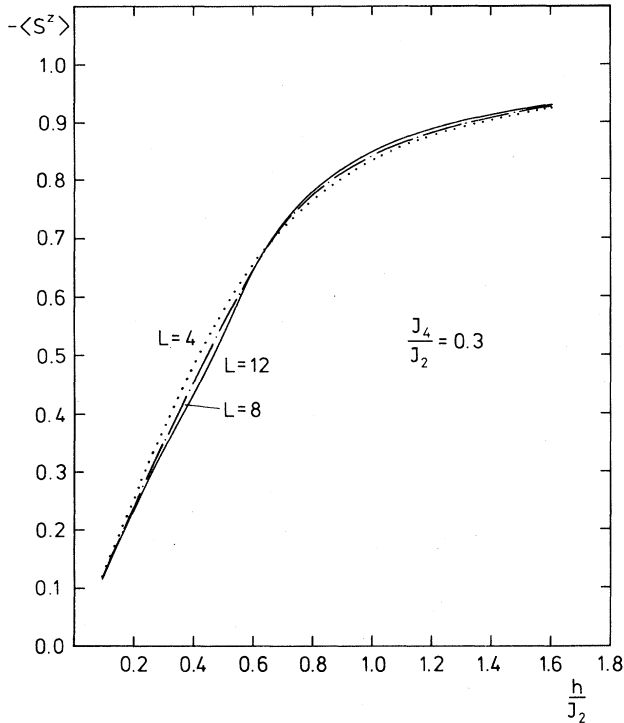


FIG. 6. Entropy of the system (2) as a function of $g = h/J_2$ for $\kappa = 0.3$ for blocks of $L = 4, 8,$ and 12 spins. The curve for $L = 16$ spins is, on this scale, practically indistinguishable from that of $L = 12$ spins.

classical system of L spins corresponds to the ground-state energy $(1/L)E_0(g, \kappa)$ of (2), then the entropy is equal to $\partial E_0(g, \kappa)/\partial g$ which in turn is equal to $-\langle 0 | S^z | 0 \rangle$.

The form of $-\langle 0 | S^z | 0 \rangle$ provides additional evidence

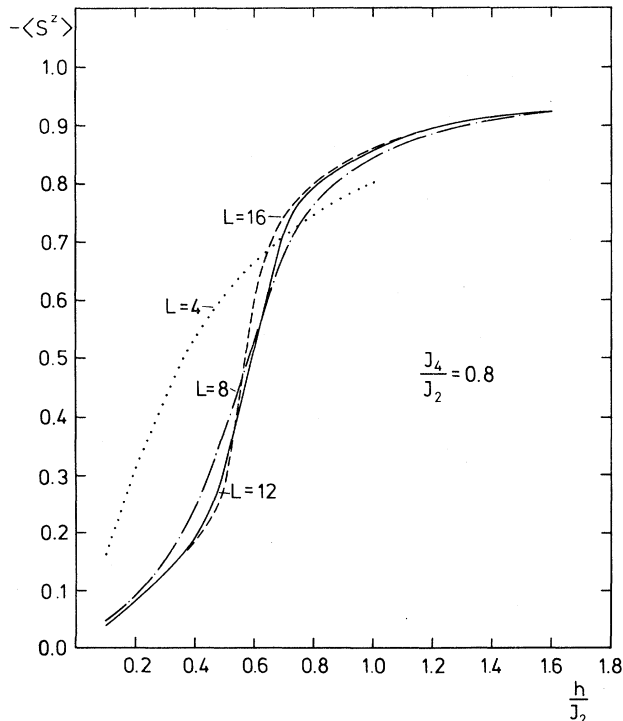


FIG. 7. Entropy of the system (2) as a function of $g = h/J_2$ for $\kappa = 0.8$ for spin blocks of sizes $L = 4, 8, 12,$ and 16 spins.

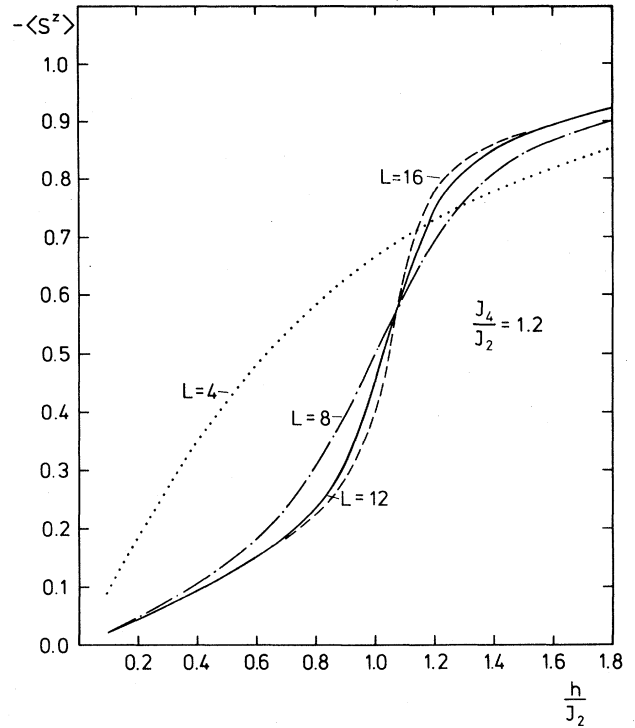


FIG. 8. Entropy of the system (2) as a function of $g = h/J_2$ for $\kappa = 1.2$ for spin blocks of sizes $L = 4, 8, 12,$ and 16 spins.

for a second-order transition for $\kappa < 0.5$ and first order otherwise. The plot of $\partial E_0(g)/\partial g$ for $\kappa = 0.3$ is representative for all $0 < \kappa < 0.5$ and is presented in Fig. 6. In Figs. 7 and 8, the same quantity is shown for $\kappa = 0.8$ and 1.2 , respectively. For $\kappa = 0.3$, there is a weak size dependence and $-\langle S^z \rangle$ seems to develop an inflection point at $g \approx 0.5$ with a weak singularity at higher derivatives and no discontinuity. This is consistent with the behavior at $\kappa = 0$ (Ising model). For $\kappa = 0.8$ (Fig. 7) a stronger size dependence can be observed, and a discontinuity appears to build up with the size at $g \approx 0.47$. In Fig. 8, an even stronger size dependence can be seen.

In Figs. 7 and 8, relatively large portions of the curves are linear in g , suggesting that the bulk entropy near the transition varies as $C_{\pm} |g - g_c|^{1-\alpha}$, where the specific-heat exponent $\alpha \approx 1$ and $C_+ \neq C_-$.

The FSS method, in general, does not give good independent estimates of α .³⁰ However, a very strong size dependence of the results for $\kappa > 0.5$ (as compared with $0 < \kappa < 0.5$) is persuasive, and when combined with the results of Sec. III this size dependence is very strongly suggestive of first-order phase transition in this region.

V. CONCLUSIONS AND DISCUSSION

The phase diagram and critical properties of the generalized 2D Ising model with anisotropic competing two- and four-body interactions was obtained by the FSS method applied to the 1D quantum representation. For $\kappa < 0.5$, the transition is of conventional 2D Ising-model type. For $\kappa > 0.6$, the transition is of first order. In the immediate neighborhood of the degeneracy point $\kappa = 0.5$ ($0.5 < \kappa < 0.6$), the FSS method does not give definite

answers due to the lack of convergence, typical for systems with very degenerate ground states as, for example, the antiferromagnetic Potts model.⁴⁰ The character of transition is consistently confirmed by an independent calculation of entropy of transition. This last quantity displays a distinctly different size dependence in second- and first-order transition regions, in accordance with general theoretical predictions.

The structure of the phase diagram (see Fig. 3) resembles, with an appropriate reinterpretation of the coupling constant κ , the phase diagram of the 2D ANNNI model. However, the characteristic thin "tongue" of the incommensurate phase of the ANNNI model does not seem to appear in the phase diagram of (2). The calculations of the gap $\Delta(q)$ for a given wave vector q do not reveal any anomalies for (2), whereas characteristic minima of $\Delta(q)$ for $q \neq \pi/2$ persist for the ANNNI model. An heuristic argument can be given showing that the four-body interaction $\sim J_4$ does not favor an incommensurate phase.⁴¹ It is based on considerations of energetics of walls. Imagine that the system (2) at $T=0$, initially in the ferromagnetic state $+++++$, formed a single wall $+++|---$. (These configurations are then repeated in a z direction.) It costs $E_{1w}=2(J_1-2J_4)$ to create one wall. One can create many walls and calculate the interaction between them. The peculiar feature of these walls is that when they get too close to each other their interaction disappears. That is, a double wall $+++|+|+++$ has precisely the energy

$E_{2w}=2E_{1w}$. One may first think that such walls would define a stripped phase with alternating $+$ and $-$ chains ($p=1$ system⁶). However, the point is that such double walls do not hang together. The energies of a "kink"

$$\begin{aligned} &++++|+|++++ \\ &+++++|+|++++, \end{aligned}$$

and a "split,"

$$\begin{aligned} &+++|+|++++ \\ &+++++|+|+, \end{aligned}$$

are equal, and the system can gain a lot of entropy by letting the walls come apart, and there is no reason why the system should choose an incommensurate phase. So the behavior can be very different from the ANNNI case.

Another feature different from the ANNNI model is the first-order character of transition for $\kappa > 0.6$. It has been conjectured from both correlation and entropy arguments. The precise nature of singularities along this line is yet to be established as well as the character of transition for $0.5 < \kappa < 0.6$.

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