Surface energy and free-boson approximation in a competing multispin model

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The phase diagram and critical behavior of a two-dimensional system with competing multispin interactions, known as the two-plus-four model, are studied by means of simple approximate analytical methods. Using the Müller-Hartmann and Zittartz approximation, the interface free-energy calculation in the ferromagnetic region is reduced to a single-particle problem. We found acceptable agreement with earlier finite-size scaling results. The model is also considered in the Hamiltonian limit, where a linearized Holstein-Primakoff transformation is used to replace spin interactions by a set of independent Bose excitations. We conjecture that the phase transition is first order when the ratio of the four-spin and nearest-neighbor interactions is greater than one-half. Standard perturbative calculations for low temperatures also indicate that the model could display first-order phase transitions.

I. INTRODUCTION

A few years ago Penson[1] suggested the convenience of introducing a new Ising-type model with competing multispin interactions as a contribution to an increasing interest in such systems in different fields.[2] There is evidence[3] of important effects of many-body interactions which naturally led to the idea that this type of force has to be included to have a more adequate description of reality than in models using only pairwise interactions. According to the exact results available,[4] it is clear that multibody forces have a strong influence on the critical behavior of model systems, introducing significant differences with the classical solution of the two-dimensional Ising model. It is natural to consider the relationship between the critical features and these types of interactions, when they are made to compete with the nearest-neighbor interaction. This has been done by Penson and Kolb[1,5] using a quantum Hamiltonian analog and by the present authors[6] in the isotropic case by means of finite-size scaling (FSS) methods.

A phase diagram obtained with a Monte Carlo technique has been published very recently.[7] The phase diagram of this model with competing multispin interactions, known as the two-plus-four model, has been found to be very similar to that of the anisotropic next-nearest-neighbor Ising (ANNNI) model,[8] with a ferromagnetic, a paramagnetic, and a commensurate phase, the latter one with an eightfold degeneracy. The main qualitative difference between both systems, insofar as the works reported in Refs. 5 and 6 are concerned, is that the two-plus-four model does not display an incommensurate phase. However, numerical approaches demand growing lattice sizes as the ratio of competing interactions increases. Moreover, most of the numerical work is based on the application to first-order phase transitions of criteria well verified only for continuous transitions; this point still needs further clarification.

In this work we adopt an alternative approach and perform different types of simple analytical calculations in an attempt to describe some features of the model, namely its phase diagram and the character of its phase transitions. The results of this article are presented in the following order. In Sec. II, we define the model, briefly review its ground-state structure, and obtain its ferromagnetic boundary via the interface approximation of Müller-Hartmann and Zittartz[9] (in the following referred to as MHZ). In Sec. III, we consider the Hamiltonian limit assuming, as usual, that anisotropy is not relevant as far as the universal properties are concerned. After a duality transformation,[10] we further simplify the row-to-row transfer matrix of the model at low temperatures by means of a linearized Holstein-Primakoff transformation.[11] We refer to this as the free-boson approximation (FBA). Although this method has been extensively used in the quantum theory of magnetism,[12] as far as we know it has not been applied to classical Ising systems via their transfer matrices.[13] We conjecture that the model undergoes first-order phase transitions and argue that if modulated phases were stable, they should be incommensurate structures for some values of the competition ratio.

In Sec. IV a standard low-temperature perturbative expansion is introduced. These calculations also indicate that the model could exhibit first-order phase transitions. Finally, in Sec. V, we make some concluding remarks.

II. THE MODEL AND ITS SURFACE ENERGY IN THE FERROMAGNETIC REGION

The two-plus-four model is characterized by the reduced Hamiltonian

$$-\beta H=\sum_{m,n}(K_0 s_{m,n}s_{m+1,n}+K_2 s_{m,n}s_{m,n+1} -K_4 s_{m,n}s_{m,n+1}s_{m,n+2}s_{m,n+3}) \quad (2.1)$$

with $\beta=1/T$. The Boltzmann constant is taken to be unity. The sums extend over the sites of a rectangular lattice with Ising spins $s_{m,n}=\pm 1$. The indices m and n correspond to the x and y directions, respectively.

We consider throughout this work $K_0,K_2,K_4>0$ and adopt the usual parametrization of the ANNNI model: $X=K_4/K_2$, which measures the degree of competition between two- and four-spin interactions. Note that K_4 should be positive definite, otherwise no competition with ferromagnetic interactions is possible.

For $X<0.5$ the ground state is ferromagnetic, while for $X>0.5$ it is an octuplet consisting of repeated patterns of spins, such that $\mathrm{sgn}(s_1s_2s_3s_4)=-1$:

$$(+---),(-+--),\ldots,(-+++)$$

along the x axis.[1] The spin arrangement along the y axis is always ferromagnetic. This phase will be denoted as $\langle 3,1\rangle$.

The rest of this section will be devoted to the evaluation of the interface free energy between two regions or domains with different ferromagnetic states. Phase transitions are then indicated by the vanishing of the interface free energy.

In a recent study of the wetting transition for the same model,[14] the phase boundary was obtained by means of the MHZ approximation, and some details of the calculation for $X>0.5$ were given. Here we develop a simple alternative technique for $X<0.5$ which gives both the ferromagnetic boundary and the eigenvalue spectrum of the transfer matrix.

MHZ assume that it is sufficient to consider only simple nonreversing interfaces (overhangs and clusters configurations are excluded in this scheme). This assumption appears to be justified in particular for large K_0 which is the case of the Hamiltonian limit. In spite of this restriction, the results are often accurate and in some cases even exact.

Following MHZ, the interface free energy per row or surface energy σ is given by

$$\sigma=T\left[2K_2(1-2X)-\lim_{N_y\to\infty}\frac{1}{N_y}\ln Z\right] . \tag{2.2}$$

The first term of the right-hand side of Eq. (2.2) is the energy needed to create a straight domain wall perpendicular to the uniaxial direction, while Z is the partition function of a lattice with N_x columns, N_y rows, and two different ferromagnetic domains. In the MHZ approximation, Z is given by

$$Z=\sum_{(n_i)}\exp[-\beta\Delta E(n_i)] , \tag{2.3}$$

where $\Delta E(n_i)$ is the energy relative to a straight wall configuration and the sum runs over all the possible wall kinks (n_i) along the N_y rows.

Then Z is written as

$$Z=\sum_{|n_1\rangle}\cdots\sum_{|n_{N_y}\rangle}\langle n_1|\hat{\theta}|n_2\rangle \times\langle n_2|\hat{\theta}|n_3\rangle\cdots\langle n_{N_y-1}|\hat{\theta}|n_{N_y}\rangle , \tag{2.4}$$

where $\hat{\theta}$ is a row-to-row transfer operator defined as

$$\langle i|\hat{\theta}|j\rangle=\exp-(2K_0d_{i,j}) . \tag{2.5}$$

State $|i\rangle$ ($|j\rangle$) corresponds to a row with a wall in the ith (jth) column and $d_{i,j}=|i-j|$ is the distance between the walls of two successive rows.

Imposing periodic boundary conditions on the lattice rows, in the thermodynamic limit Z is simply

$$Z=(\lambda_{\max})^{N_y} , \tag{2.6}$$

where $\lambda_{\max}$ is the maximum eigenvalue of $\hat{\theta}$.

Now, any single-wall row configuration $|n\rangle$ may be associated with a single-particle state

$$c_n^{\dagger}|\mathrm{vac}\rangle=|n\rangle , \tag{2.7}$$

where $|\mathrm{vac}\rangle$ is the state with zero particles (or walls). The transfer matrix then takes the form of a single-particle problem, namely

$$\hat{\theta}=\sum_j\sum_d\gamma_0^d(c_j^{\dagger}c_{j+d}+\mathrm{H.c.}) \tag{2.8}$$

with $\gamma_0=\exp-2K_0$, $d=0,1,2,\ldots$.

By Fourier transforming, the diagonalization of $\hat{\theta}$ is now immediate and is written down as

$$\hat{\theta}=\sum_k\lambda_kc_k^{\dagger}c_k , \tag{2.9}$$

where

$$\lambda_k=\frac{1-\gamma_0^2}{\gamma_0^2+1-2\gamma_0\cos k} , \tag{2.10}$$

from which it follows that

$$\lambda_{\max}=\lambda_{k=0}=\coth K_0 . \tag{2.11}$$

Then the surface energy associated with the coexistence of two ferromagnetic domains is given by

$$\sigma=T[2K_2(1-2X)+\ln(\tanh K_0)] . \tag{2.12}$$

The ferromagnetic phase boundary obtained by setting $\sigma=0$ is

$$\sinh[2K_2(1-2X)]\sinh 2K_0=1 . \tag{2.13}$$

This is indicated in Fig. 1, where satisfactory agreement with earlier FSS results is observed. As usual, this type of calculation gives the correct surface energy and transition line of the ordinary Ising model ($X=0$).

An immediate generalization of this calculation to similar models with M spins (M even) interactions (K_M) in one direction can be done. The ferromagnetic phase boundary of such models is computed similarly and is found to be

$$\sinh(2K_2-MK_M)\sinh 2K_0=1 . \tag{2.14}$$

For all M, the phase transition turns out to be continuous.

In the next section we turn to a different kind of approximation.

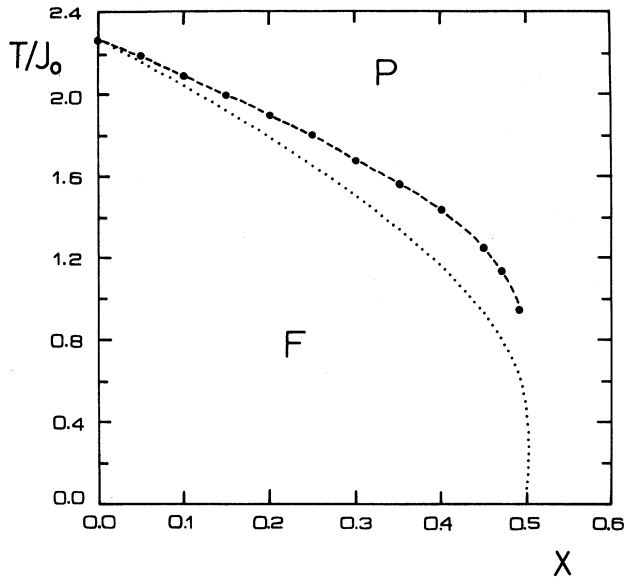

FIG. 1. Ferromagnetic phase boundary. The dotted line is the boundary obtained with the MHZ approximation for $K_2=K_0=J_0/T$. Solid circles denote previous finite-size scaling results (Ref. 6).

III. FREE-BOSON APPROXIMATION IN THE HAMILTONIAN LIMIT

Starting from the Hamiltonian model, the row-to-row transfer matrix is easily written down (omitting an innocuous factor $[2\sinh 2K_0]^{N_x/2}$) as

$$V=\exp\left[K_0^*\sum_n \eta_n^x\right]\exp\left[K_2\sum_n \eta_n^z\eta_{n+1}^z - K_4\sum_n \eta_n^z\eta_{n+1}^z\eta_{n+2}^z\eta_{n+3}^z\right], \tag{3.1}$$

where $tgh K_0^*=\exp(-2K_0)$ and the Pauli matrices η_n^x and η_n^z act on the nth spin of a given row. The thermodynamic functions and different correlation functions can be expressed in terms of the eigenvalues and eigenvectors of V.

Since V is difficult to handle in its present form, let us consider the Hamiltonian limit, where the transfer matrix is written in terms of a single exponential argument. Formally this is correct if $K_2,K_4,K_0^*\ll 1$, which corresponds to strong coupling in the vertical and weak coupling in the horizontal direction. Then the transfer matrix is written as $V=\exp(-H)$, where

$$H=-K_2\sum(\eta_n^z\eta_{n+1}^z - X\eta_n^z\eta_{n+1}^z\eta_{n+2}^z\eta_{n+3}^z+\tau\eta_n^x), \tag{3.2}$$

with $\tau\equiv K_0^*/K_2$.

It will turn out that it is convenient to work with dual variables. Under the dual transformation, the Pauli operators transform according to

$$\sigma_n^x=\eta_n^z\eta_{n+1}^z,\qquad \sigma_n^z=\prod_j^{n-1}\eta_j^x . \tag{3.3}$$

For $X<0.5$, the low-temperature twofold degenerate ferromagnetic ground state of the original model is mapped into a single state representing the disordered high-temperature region of the dual model. This state corresponds to all dual spins pointing in the x direction. For $X>0.5$, the eightfold degenerate $\langle 3.1\rangle$ phase is projected into a fourfold degenerate antiphase equal to the usual $\langle 2\rangle$ phase of the ANNNI model, which is characterized by a two-spin-up–two-spin-down row configuration pointing in the x direction. The paramagnetic phase corresponds to a ferromagnetic one.

After the $\sigma_n^x\to\sigma_n^z,\sigma_n^z\to-\sigma_n^x$ transformation, the dual Hamiltonian is given by

$$H_D=-K_2\sum_n(\sigma_n^z - X\sigma_n^z\sigma_{n+2}^z+\tau\sigma_n^x\sigma_{n+1}^x) . \tag{3.4}$$

The advantage of H_D over H is that it does not contain four-spin interactions.

Now we introduce boson operators via the Holstein-Primakoff transformation, which for spins one-half reads

$$\sigma_n^+=(1-\mu_n^\dagger\mu_n)^{1/2}\mu_n ,\qquad \sigma_n^-=\mu_n^\dagger(1-\mu_n^\dagger\mu_n)^{1/2} ,\qquad \sigma_n^z=1-2\mu_n^\dagger\mu_n . \tag{3.5}$$

Here, σ_n^+ and σ_n^- are spin raising and lowering operators and the μ's are operators which exactly satisfy boson commutation relations. Different ground-state structures of H_D have to be considered separately.

A. $X<0.5$

In this case we can linearize the transformation by assuming that for small τ ("temperature") the fraction of spins deviating from their ferromagnetic ground state is negligible. As it will be shown, this assumption works properly even very near the transition point τ_c.

Then Eq. (3.5) is rewritten as

$$\sigma_n^+=\mu_n,\quad \sigma_n^-=\mu_n^\dagger,\quad \sigma_n^z=1-2\mu_n^\dagger\mu_n . \tag{3.6}$$

Finally, of course, as $\tau\to\tau_c$, the ferromagnetic ground state will become unstable and this approximation scheme breaks down. The ground-state expectation value of $(\sigma^x)^2$ arising from Eq. (3.6) is (incorrectly) equal to 2. Hence,[15] we include in what follows a factor $2^{-1/2}$ in σ^+ and σ^-.

Retaining only bilinear terms and Fourier transforming, H_D can be written as $H_D=E_0+H_0$, where

$$E_0=-K_2N_x(1-X)\quad\text{(zeroth perturbation order)}, \tag{3.7}$$

$$H_0=K_2\sum_{0<k<\pi}[2(1-2X)-\tau\cos k](\mu_k^\dagger\mu_k+\mu_{-k}^\dagger\mu_{-k}) - K_2\tau\sum_{0<k<\pi}\cos k(\mu_k^\dagger\mu_{-k}^\dagger+\text{H.c.})$$

and $\mu_k^\dagger$ creates spin-wave-like excitations, namely the Fourier transform of the quasiboson operators $\mu_n^\dagger$.

As it is known, H_0 can be diagonalized using a Bogolyubov-Valatin[16] transformation. Then H_D is rewritten in terms of new boson excitations as

$$H_D=\sum_{-\pi<k<\pi}(b_k^\dagger b_k+\tfrac{1}{2})\omega_k-\tfrac{1}{2}\sum_{-\pi<k<\pi}\alpha_k+E_0 \tag{3.8}$$

with

$$\omega_k=2K_2u\left[1-\frac{1}{u}\tau\cos k\right]^{1/2},$$
$$\alpha_k=2K_2\left[u-\frac{1}{2}\tau\cos k\right], \tag{3.9}$$
$$u=1-2X .$$

Hence the mass gap or inverse correlation length, defined as the gap between the ground and first excited states of H_D, is simply

$$\Delta=2K_2u(1-\tau/u)^{1/2} . \tag{3.10}$$

From the vanishing of the mass gap at $\tau_c=1-2X$, we recover the ferromagnetic boundary previously obtained with the MHZ method. The critical wave vector resulting from this continuous transition is always zero.

It is found that the singular part of the free energy, f^*, satisfies a scaling relation given by

$$f^*(\lambda\tau_c,\lambda\tau)=\lambda f^*(\tau_c,\tau) . \tag{3.11}$$

This scaling property will no longer be valid if $X>0.5$.

For completeness, it is worthwhile to test the validity of the approximation made in Eq. (3.6), by calculating the mean value of the quasiboson occupation number in the b's vacuum. After some simple algebraic calculations, $\langle\mu^\dagger\mu\rangle$ is found to be

$$\langle\mu^\dagger\mu\rangle=\frac{E(p)+p^2K(p)}{\pi(1+p^2)^{1/2}}-\tfrac{1}{2} \tag{3.12}$$

with

$$p=(\tau_c/\tau)-[(\tau_c/\tau)^2-1]^{1/2} , \tag{3.13}$$

and $K(p),E(p)$ the complete elliptic integrals of the first and second kind, respectively.[17] It is interesting to note that even at $\tau=0.99\tau_c$, the average of $\mu^\dagger\mu$ is less than 0.1, i.e., the linear scheme is still an acceptable approximation.

B. $X>0.5$

Although the algebra involved in this case is simple and similar to the former case, it demands a lengthy calculation due to the ground-state structure. After retaining only bilinear terms and using a Tyablikov[18] transformation to decouple the eight resulting modes (see the Appendix for calculation details), we finally obtain the elementary excitations of H_D which always display a nonvanishing gap. Here, we will adopt an *ad hoc* criterion and assume that when the mass gap reaches a finite minimum (maximum correlation length), the system has a first-order phase transition. At low temperatures the resulting phase boundary is, as expected, in acceptable agreement with earlier FSS calculations.[1] In Fig. 2 we show the phase diagram obtained using the free-boson approximation compared to numerical data.

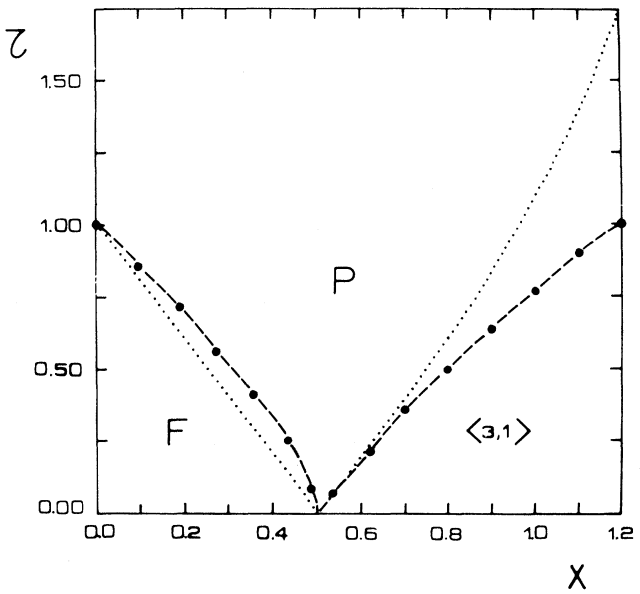

FIG. 2. Phase diagram of the two-plus-four model in the Hamiltonian limit, obtained using the free-boson approximation (dotted line). We also show the results obtained by Penson (Ref. 1) using finite-size scaling (solid circles).

It also turns out that if $X>0.5$, the energetics of the system in the thermodynamic limit may impose a critical wave length which is not commensurable with the period of the chain. This result does not necessarily imply the existence or stability of modulated phases, although if this were the case, they should display an incommensurate structure for certain competition ratios. Although these results are not conclusive, nevertheless they are useful to indicate that the physical behavior underlying the region $X>0.5$ is rather different from that corresponding to the ferromagnetic case.

IV. PERTURBATIVE CALCULATIONS

The main problem in applying standard perturbation theory at small τ is that the degeneracy of the ground state of H cannot be removed in any order of perturbation even if $X\neq0.5$. From a practical point of view it is reasonable to avoid such complication by using the dual representation H_D.

The unperturbed problem for small τ is

$$H_0=-K_2\sum_n(\sigma_n^z-X\sigma_n^z\sigma_{n+2}^z)\ , \tag{4.1}$$

while the (even) perturbation is given by

$$V=-K_2\tau\sum_n\sigma_n^x\sigma_{n+1}^x\ . \tag{4.2}$$

We shall compute the mass gap of H_D up to third order in τ, because for $X>0.5$ this is the lowest order which removes the translational invariance degeneracy of the first excited state.

First we consider the case $X<0.5$ which is characterized by a ferromagnetic ground state. After a straightforward calculation, the third-order mass gap is found to be

$$\Delta_k^{(3)}=K_2\left[2(1-2X)-2\tau\cos k+\frac{\tau^2\sin^2k}{(1-2X)}+\frac{\tau^3}{(1-X)^2}\left[\frac{X(1-X)\cos k}{(1-2X)^2}+\tfrac{1}{2}\cos^3k-\tfrac{3}{8}\cos 3k\right]\right]\ . \tag{4.3}$$

It follows from this expression that the whole perturbation scheme is singular at $X=0.5$, which is not so surprising in view of the infinite degeneracy of the ground state at $\tau=0$, $X=0.5$. The first-order correction leads to the ferromagnetic boundary previously obtained using the MHZ and the free-boson approximation methods; the critical wave vector is always zero.

A rather different critical behavior is found in second and third order. In the latter case, for $X\gtrsim 0.17$ there is a nonvanishing mass gap at low temperatures; we interpret this result as in Sec. III, i.e., we assume the system has a first-order phase transition, which implies that there should be a tricritical point at this value of X.

Minimizing Eq. (4.3) it is found that for $X<0.46$ the resulting third-order wave vector is zero. Above this value of X, the third-order boundary becomes unstable, as expected when $X\to 0.5$. Similar results were obtained for second-order corrections.

We now consider the case $X>0.5$, characterized by a ground state equal to the usual $\langle 2\rangle$ phase of the ANNNI model. We found that the third-order mass gap is given by

$$\Delta_k^{(3)}=K_2\left[4X-2-\tau-\frac{1}{2}\tau^2\left[\frac{1}{4X}-\frac{1}{2X+1}+\frac{1}{1+X}-\frac{1}{2(2X-1)}+\frac{1}{2}\right]-\frac{1}{8}\tau^3\left[\frac{1}{X}+\frac{1+\cos k-9/4}{2X^2}\right]\right]\ , \tag{4.4}$$

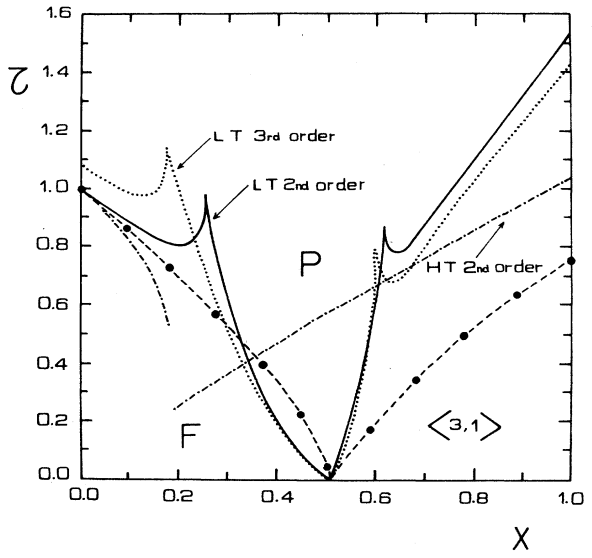

FIG. 3. Phase diagram of the two-plus-four model in the Hamiltonian limit, obtained using low- and high-temperature expansions. The solid and dotted lines represent the second- and third-order terms of the low-temperature expansion, respectively; the dashed line indicates the second-order term of the high-temperature expansion. As before, solid circles indicate Penson's results (Ref. 1). We do not show first-order results separately, to improve clarity.

from which it follows that the third-order correction is the lowest order needed to remove the translational invariance degeneracy; the resulting critical wave vector is always zero.

Below $X\simeq 0.6$ the second- and third-order gaps do not vanish. As it was previously mentioned, we then assume that the $\langle 3.1\rangle$ phase boundary arises from a first-order phase transition. Results for $X>0.6$ seem to indicate that the transition should be continuous. This calculation, however, is not too reliable because it corresponds to the region $\tau_c>1$.

A high-temperature perturbation expansion seems to be less useful, because the interesting region of the phase diagram corresponds to $\tau^{-1}>1$. If, nevertheless, one carries out this calculation, it is somewhat remarkable that the anomaly observed in the low-temperature expansion near $X=0.17$ is still present. In Fig. 3 we show the phase diagram obtained with low- and high-temperature expansions together with FSS data.

V. FINAL COMMENTS

In this work we have made three simple analytical approximations to the two-plus-four model which is an interesting example of a system with multispin interactions and modulated phases. In what follows we make some final comments in addition to those made in previous sections.

By now it is well established that a continuous transition can be detected by the vanishing of the corresponding mass gap of the equivalent quantum Hamiltonian version. To our knowledge there is no similar result in relation to the first-order phase transitions (which, as is well known, are characterized by a nondivergent correlation length). In this paper (see Secs. III and IV), we have used as a criterion that a (finite) minimum in the energy gap corresponds to a first-order phase transition. *A posteriori,* we found that in the FBA this assumption is in good agreement with published numerical results.

The free-boson and MHZ approximations led to the same ferromagnetic boundary and predicted a continuous phase transition along it. Indeed, first-order low-temperature perturbation theory yields the same result. This agreement, however, is lost when higher-order corrections are considered: in this case the phase transition ceases to be continuous for $X>0.17$ and the phase boundary is somewhat changed. We want to emphasize that the anomaly seen in Fig. 3 around this tricritical point needs further study. We found it suggestive that in the ANNNI model there seems to be an anomaly at almost the same value of the competition ratio:[19] it is not unreasonable to think that it could be a similar origin for this behavior in both models (like, for instance, the presence of the disorder line).

The FBA turns out to be surprisingly good for values of X which are not too large, up to "temperatures" very near τ_c. In the critical region, however, a more reliable calculation should keep higher-order terms of Eq. (3.5).

It is interesting to remark that H_D, within the approximation given by Eq. (3.7), does not conserve the number of particles; its ground state is a linear combination of states with a variable number of pairs of particles with momentum $(k,-k)$. In this sense, it is analogous to the BCS ground state of superconductivity.

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APPENDIX

The purpose of this appendix is to describe some details of the free-boson approximation in the region $X>0.5$. Let us consider the four sublattices obtained by keeping one of every four columns of the original lattice, and associate to each sublattice site a Pauli spin operator in the following way:

$\sigma_{4n+p}=\sigma_{s,n}$ *with* $s=a,b,c,d$ according to $p=1,2,3,4$, respectively; $N=1,2,\ldots,N_x/4-1$.

The linearization of Eq. (3.5) now appears as

$$\sigma^{+}_{a,n}=a_n,\quad \sigma^{+}_{b,n}=b_n,\quad \sigma^{+}_{c,n}=c^{\dagger}_n,\quad \sigma^{+}_{d,n}=d^{\dagger}_n\ . \tag{A1}$$

By Fourier transforming and retaining only bilinear terms, H_D is written as $H_D=E_0+H_0$, with

$$\begin{aligned}
&E_0=-N_xXK_2 \text{ (zeroth perturbation order)}\ ,\\
&H_0=-K_2\Big[2u\sum_{-\pi<k<\pi}(c^{\dagger}_kc_k+d^{\dagger}_kd_k)-2v\sum_{-\pi<k<\pi}(a^{\dagger}_ka_k+b^{\dagger}_kb_k)\\
&\quad+\tau\sum_{-\pi<k<\pi}(a^{\dagger}_kb^{\dagger}_{-k}+a^{\dagger}_kb_k+\text{H.c.})+\tau\sum_{-\pi<k<\pi}(c^{\dagger}_kd_{-k}+c^{\dagger}_kd_k+\text{H.c.})\\
&\quad+\tau\sum_{-\pi<k<\pi}(b^{\dagger}_kc^{\dagger}_{-k}+b^{\dagger}_kc_k+\text{H.c.})+\tau\sum_{-\pi<k<\pi}(e^{ik}d^{\dagger}_ka^{\dagger}_{-k}+e^{-ik}d^{\dagger}_ka_k+\text{H.c.})\Big]\ ,
\end{aligned} \tag{A2}$$

where $v=(1+2X)$ and u is defined as in Eq. (3.9). In spite of the apparent difficulty of this expression, it is bilinear and can be diagonalized with the help of a generalized Bogolyubov transformation introduced by Tyablikov[18] in the quantum theory of magnetism.

In each k subspace there are eight kinds of excitations and from a practical point of view it is convenient to relabel them in the following way:

$$\begin{aligned}
&a_k=B_{1,k},\quad b_k=B_{2,k},\quad c_k=B_{3,k},\quad d_k=B_{4,k}\ ,\\
&a_{-k}=B_{5,k},\quad b_{-k}=B_{6,k},\quad c_{-k}=B_{7,k},\quad d_{-k}=B_{8,k}\ .
\end{aligned} \tag{A3}$$

With this notation, H_D is decomposed in 8×8 blocks which in turn are expanded in three types of processes:

$$H=H_1(B^{\dagger}B)+H_2(B^{\dagger}B^{\dagger})+H_3(BB)\ , \tag{A4}$$

where

$$\begin{aligned}
&H_1=\sum L_{\alpha,\beta}B^{\dagger}_{\alpha}B_{\beta}\ ,\\
&H_2=\tfrac{1}{2}\sum_{\alpha,\beta}M_{\alpha,\beta}B^{\dagger}_{\alpha}B^{\dagger}_{\beta}\ ,\\
&H_3=\tfrac{1}{2}\sum_{\alpha,\beta}M^{*}_{\alpha,\beta}B_{\alpha}B_{\beta}\ .
\end{aligned} \tag{A5}$$

Here, L and M are, respectively, Hermitian and symmetric matrices, written as

$$L=\begin{bmatrix}F_k & 0\\ 0 & F_{-k}\end{bmatrix},\quad M=\begin{bmatrix}0 & R_{-k}\\ R & 0\end{bmatrix}\ , \tag{A6}$$

where F_k and R_k are 4×4 Hermitian matrices given by

$$F_k=-K_2\tau\begin{bmatrix}-2v/\tau & 1 & 0 & e^{ik}\\ 1 & -2v/\tau & 1 & 0\\ 0 & 1 & 2u/\tau & 1\\ e^{-ik} & 0 & 1 & 2u/\tau\end{bmatrix},$$

$$R_k=-K_2\tau\begin{bmatrix}0 & 1 & 0 & e^{ik}\\ 1 & 0 & 1 & 0\\ 0 & 1 & 0 & 1\\ e^{-ik} & 0 & 1 & 0\end{bmatrix}. \tag{A7}$$

Now we perform the Tyablicov canonical transformation from quasiboson operators B to new operators T

$$T_\mu=\sum_\alpha (x_{\mu\alpha}B_\alpha-y_{\mu\alpha}B_\alpha^\dagger)\ , \tag{A8}$$

which almost satisfy boson commutation relations provided that

$$\begin{aligned}&\sum_\alpha (x_{\mu\alpha}x^*_{\nu\alpha}-y_{\mu\alpha}y^*_{\nu\alpha})=\delta_{\mu\nu}\ ,\\ &\sum_\alpha (x_{\mu\alpha}x_{\nu\alpha}-y_{\mu\alpha}y_{\nu\alpha})=0\ .\end{aligned} \tag{A9}$$

Using Eq. (A9) we can find the inverse transformation of Eq. (A8), which turns out to be

$$B_\alpha=\sum_\mu (x^*_{\mu\alpha}T_\mu+y^*_{\mu\alpha}T_\mu^\dagger)\ . \tag{A10}$$

Taking into account Eq. (A10) and the solution of the secular problem $[H,T_\alpha]=\omega_\alpha^{(k)}T_\alpha$, the elementary excitations $\omega_\alpha^{(k)}$ are finally derived from the positive eigenvalues of an 8×8 matrix Ω_k given by

$$\Omega_k=\begin{bmatrix}F_k & R_{-k}\\ R_{-k} & -F_k\end{bmatrix}. \tag{A11}$$

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$$(\sigma_n^x)^2=(\mu_n^\dagger+\mu_n)^2=1+2\mu_n^\dagger\mu_n+(\mu_n^\dagger)^2+(\mu_n)^2\ .$$

The ground-state expectation value of $(\sigma_n^x)^2$ is 2, rather than the correct value 1. To correct this discrepancy we used "renormalized" operators

$$\sigma_n^+=2^{-1/2}\mu_n,\quad \sigma_n^-=2^{-1/2}\mu_n^\dagger\ ,$$

retaining $\sigma_n^z=1-2\mu_n^\dagger\mu_n$ as the dual order parameter; then we obtain the correct ground-state expectation value.

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