Generalized boundary conditions for periodic lattice systems: Application to the two-dimensional Ising model on a square lattice

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(Received 20 May 2004; published 23 December 2004)

We show that the thermal properties of periodic lattice systems can be approximated to that of a finite cluster with appropriate boundary conditions which include a modified Hamiltonian for the boundary variables. Imposing lattice invariance on the correlation of the local site variables is sufficient to obtain the free parameters of the boundary Hamiltonian. The degree of accuracy of the calculation depends on the interaction range allowed in the boundary Hamiltonian and the range up to which the correlation of the site variables are made lattice invariant. The Bethe approximation can be considered a trivial case of this general method for clusters of one lattice site. The reliability of the method is demonstrated with the results obtained for the two-dimensional Ising model, where a cluster of four spins and invariance conditions up to second neighbors is sufficient to reproduce some nonuniversal thermal properties of the model with an accuracy comparable or better than other more complex numerical methods.

DOI: 10.1103/PhysRevE.70.066133 PACS number(s): 05.50.+q, 05.10.−a

I. INTRODUCTION

Among the many Hamiltonian models of phase transitions very few have been solved exactly, and the use of efficient approximation methods is crucial; they have to be accurate enough and maintain the computational effort under some practical limits. A considerable effort has been devoted to this task: from the easy to implement mean-field theory to sophisticated series expansions and renormalization techniques, going through Monte Carlo or molecular dynamic simulations [1,2]. Those approaches differ on the complexity of calculations and accuracy of the results, but from a very basic point of view some of them share common features. Monte Carlo simulations and mean-field calculations, for instance, look completely different, but the most relevant distinction is the way in which the pertinent statistical sums are performed. In both cases the infinite system is approached by a finite cluster, appropriate boundary conditions are used, and thermodynamic magnitudes are calculated. Often, within the mean-field approach, the number of relevant thermodynamic variables in the cluster is so small that sums may be calculated within almost any desired accuracy, and the best-suited boundary conditions correspond to a fixed self-consistent value of the order parameter. In Monte Carlo simulations, the number of degrees of freedom is so large that the sums must be calculated by means of a statistical sampling in the phase space of the system, and usually, periodic boundary conditions are implemented, although there is no conceptual problem to use self-consistent fields at the boundary of a Monte Carlo simulation [3,4]. In the simplest version of mean-field theory [5], correlations among the boundary variables and correlations between the cluster and boundary are neglected. The first step towards the use of more adequate boundary conditions—the boundary variables are allowed to fluctuate—correspond to the well-known Bethe [6] approximation, where correlation effects are implicitly taken into account. On the other hand, periodic boundary conditions overestimate the correlations among all the variables, especially when the correlation length and the size of the system are of the same order of magnitude. Hence the discussion may be rephrased in the following way: Which are the best boundary conditions that lead the variables in a finite cluster to behave as if they were in the infinite ideal system?

Significant efforts have been made in the development of cluster-based methods. Starting from the mean-field or Bethe approximation, the most straightforward approach consists in increasing the size of the cluster, maintaining the characteristics of the boundary conditions. Unfortunately, the translational invariance of the lattice is violated [7], and the convergence to the thermodynamic limit is slow. The convergence problem may be highly improved [8] analyzing the results by the coherent-anomaly method [9–15], that allows us to extract nonclassical critical exponents and transition temperatures from convergent series of mean-field approximations. The lack of periodicity has been studied in Ref. [7], and a different self-consistent mean-field equation has been proposed. This approach predicts with great accuracy the transition temperatures in low dimensional spin systems. Other approximations such as the effective-field model [16] and its extensions [17–19], the double-chain approximation [20], or the cluster-variation method [21–25] are designed to treat correlations more accurately, and constitute a significant improvement over the simple Weiss theory. One of the drawbacks of the usual methods is that they are de-

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signed to study discrete models, and their extension to continuous variables is often difficult or unfeasible. The different kind of boundary conditions proposed in this work exhibit two interesting features: first, as correlations are more accurate, the statistical behavior of the finite system resembles more closely that of the infinite one; second, its applicability is, in principle, not restricted to discrete models.

The application of more complex effective couplings to the boundary spins of a given cluster has also been studied by Minami *et al.* in the multi-effective-field theory [26] from the viewpoint of the coherent anomaly method. Although the present work is not focused as this one on universal quantities at the transition point but on the whole behavior of the model within large temperature intervals, both methods are somehow similar: the effective interactions go beyond nearest-neighbor couplings, and the consistency equations contain *n*-body correlation functions. In this work, however, the couplings are added in a systematic manner, and more crucial, the whole cluster is periodic within a given level of accuracy. In Ref. [26] not all the symmetry equivalent *n*-body correlation functions are forced to be equal, and the cluster, from this viewpoint, does not satisfy the periodicity conditions.

Although the basis of the method is completely general, its foundations (Sec. II) and application (Sec. III) are explained in the context of the two-dimensional Ising model in a square lattice. This system has been chosen for practical reasons. On the one hand, the model is simple compared to other models of cooperative phenomena, and the calculation of the statistical averages is not very time consuming. On the other hand, the model is rich enough to exhibit a phase transition at finite temperature, and the behavior of several statistical magnitudes has been calculated exactly [27–29]. These exact solutions give us an appropriate basis to estimate the accuracy of the method in calculations of nonuniversal quantities such as critical temperatures and maximum values of connected correlation functions.

II. PERIODICITY AND BOUNDARY CONDITIONS

In the absence of external field, the Hamiltonian of the Ising model in a two-dimensional square lattice may be expressed as

$$H = -J\sum_{\langle i,j\rangle}\sigma_i\sigma_j,$$

where the sum extends to all the nearest-neighbor pairs and the available values of the spin variables are $\sigma = \pm 1$. We can divide the whole system in three sets of spins (Fig. 1): a small cluster of spins (C spins, $\sigma_i^c \in C$), the spins that interact with the cluster, located at the boundary (B spins, $\sigma_i^b \in B$), and the spins that are neither in the cluster, nor in its boundary, i.e., the rest of the spins (R spins, $\sigma_i^r \in R$). The number of spins at the boundary depends on the range of the interactions, and in this case only the first neighbors of the cluster spins have to be taken into account. The density matrix of the whole system is given by

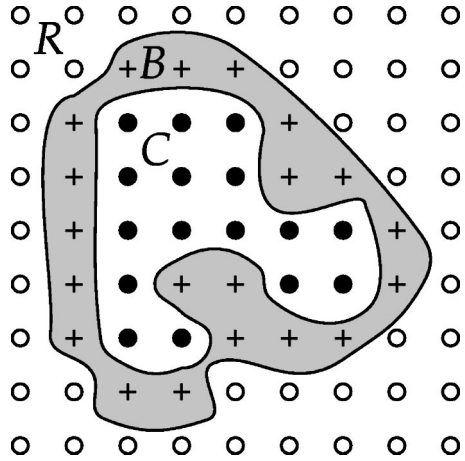

FIG. 1. Schematic view of a two-dimensional Ising system in a square lattice. Filled circles correspond to the spins in the cluster (σ_i^c). The boundary spins (σ_i^b) are in the shadowed region, and the open circles correspond to the rest of the infinite system (σ_i^r).

$$\rho(\{\sigma^c,\sigma^b,\sigma^r\}) = \frac{1}{Z}\exp[-\beta H(\{\sigma^c,\sigma^b,\sigma^r\})], \tag{1}$$

where $Z = \mathrm{tr}\exp[-\beta H]$ is the partition function, and $\{\sigma^c,\sigma^b,\sigma^r\}$ represents a given statistical configuration of the spins. The reduced density matrix for the cluster and boundary spins may be obtained taking the trace over the spins of the rest of the system (R):

$$\rho(\{\sigma_i^c,\sigma_i^b\}) = \frac{1}{Z}\mathrm{tr}_R\exp[-\beta H]. \tag{2}$$

Let us create a defect by removing all the interactions between the cluster and boundary spins; the cluster becomes isolated from the boundary spins and the rest of the system, and periodicity is lost. The reduced density matrix for the C and B spins may be decomposed as

$$\rho'(\{\sigma^c,\sigma^b\}) = \rho_c'(\{\sigma^c\})\rho_B'(\{\sigma^b\}), \tag{3}$$

where the primes refer to the defective system, and ρ_C' and ρ_B' denote the reduced density matrix of the C and B spins, respectively:

$$\rho_C'(\{\sigma^c\}) = \frac{1}{Z_C'}\exp[-\beta H_C(\{\sigma^c\})], \tag{4}$$

$$\rho_B'(\{\sigma^b\}) = \frac{1}{Z_B'}\mathrm{tr}_R\exp[-\beta H_{B,R}(\{\sigma^b,\sigma^r\})]. \tag{5}$$

$H_C(\{\sigma^c\})$ is the part of the Hamiltonian that contains only the interactions among the C spins (nearest neighbor pairs of the form $\sigma^c\sigma^c$), and $H_{B,R}(\{\sigma^b,\sigma^r\})$ corresponds to the remaining interactions after isolating the two subsystems (nearest neighbor pairs of type $\sigma^b\sigma^b$, $\sigma^b\sigma^r$, and $\sigma^r\sigma^r$).

If the cluster is small, $\rho_C'(\{\sigma^c\})$ may be easily calculated. On the other hand, in $\rho_B'(\{\sigma^b\})$ the effect of the R spins is implicitly included, and, due to the lack of periodicity, its calculation is more complex than the calculation of the density matrix of the periodic infinite lattice [Eq. (1)]. The prob-

ability densities of the cluster and boundary spins in the periodic [Eq. (2)] and defective [Eq. (3)] systems may be related according to

$$\rho(\{\sigma^c,\sigma^b\}) = A^{-1}\rho'(\{\sigma^c,\sigma^b\})\exp[-\beta H_{B-C}(\{\sigma^c,\sigma^b\})], \quad (6)$$

where H_{B-C} corresponds to the interactions between the B and C spins—those that are absent in the defective system—and A is a normalization factor:

$$A = \mathrm{tr}_{C,B}\rho'(\{\sigma^c,\sigma^b\})\exp[-\beta H_{B-C}(\{\sigma^c,\sigma^b\})].$$

Using Eqs. (3) and (4) in Eq. (6), we obtain the following exact expression for the infinite ideal lattice:

$$\rho(\{\sigma^c,\sigma^b\}) = \rho'_B(\{\sigma^b\}) \times \frac{1}{AZ'_C}\exp\{-\beta[H_C(\{\sigma^c\}) + H_{B-C}(\{\sigma^b,\sigma^c\})]\}, \quad (7)$$

establishing a relationship between the reduced density matrix of the boundary spins in the defective lattice and the exact reduced density matrix of boundary and cluster spins in the ideal lattice. Thus the knowledge of the exact density matrix $\rho'_B(\{\sigma^b\})$ of the defective system is enough to obtain the exact probability density of the infinite periodic lattice; but, as mentioned above, due to the lack of periodicity, any calculation in the defective system should at least be as difficult as its counterpart in the infinite periodic lattice.

The main difficulty to apply Eq. (6) in statistical calculations relies on having a good approximation for the statistical distribution of the boundary spins in the defective system. One can generate a trial density matrix $\rho'_{B,t}(\{\sigma^b\})$ and estimate the goodness of the choice. We propose a simple criterion based on the periodicity. According to Eq. (6) the exact $\rho'_B(\{\sigma^b\})$ density of the defective system gives the exact density matrix of both cluster and boundary spins in the infinite periodic system—a periodic density matrix. Therefore the more reliable the trial distribution is, the "more periodic" is the density matrix of the cluster and boundary spins calculated by Eq. (6). The generation of the trial density matrix and the estimation of the periodicity are explained below.

A. Probability density of the boundary spins

An appropriate probability density distribution for the boundary spins must be parametrized in a simple form to allow a practical use of Eq. (6), and must contain the necessary ingredients to mimic the effect of the part of the system that is not explicitly taken into account—the R spins. A straightforward approach consists of using a trial Hamiltonian for the boundary spins, and generating the probability density distribution by

$$\rho'_{B,t}(\{\sigma^b\}) = \frac{1}{Z'_t}\exp[-\beta H^b_t(\{\sigma^b\})]. \quad (8)$$

In its simplest form H^b_t may be composed of interactions with effective fields, and quadratic couplings between pairs of spins [30]:

$$H^b_t = -J\sum_{\langle i,j\rangle}\sigma^b_i\sigma^b_j - \sum_i h_i\sigma^b_i - \sum_{i,j}K_{i,j}\sigma^b_i\sigma^b_j, \quad (9)$$

where the first summation corresponds to the part of the total Hamiltonian that involves interactions between nearest neighbors at the boundary, and in the third term there is no restriction on the distance between the spin pairs. The Hamiltonian parameters may be chosen systematically, first of all the effective fields (h_i), and afterwards, interactions covering increasing distances ($K_{i,j}$) may be taken into account: couplings between first neighbors, second neighbors, and so on. The number of independent parameters depends on the cluster size and symmetry, and the degree of periodicity that is intended to be fulfilled. As explained below, the achievement of a better degree of periodicity corresponds to an increase in the number of parameters in the trial Hamiltonian; for a low degree of periodicity most of the $K_{i,j}$ may be absent and only short distance couplings are needed.

Equations (6) and (9) may be written in a more practical and intuitive way. The trial density for spins in the boundary and cluster is

$$\rho_t(\{\sigma^c,\sigma^b\}) = \frac{1}{Z_t}\exp[-\beta(H_0 + \Delta H)], \quad (10)$$

where H_0 corresponds to the part of the Hamiltonian that does not contain spins of the rest of the system:

$$H_0 = -J\sum_{\langle i,j\rangle}\sigma_i\sigma_j \quad \forall\ \sigma \notin R, \quad (11)$$

ΔH contains the parametrized interactions that should reproduce the effect of the rest of the system:

$$\Delta H = -\sum_i h_i\sigma^b_i - \sum_{i,j}K_{i,j}\sigma^b_i\sigma^b_j, \quad (12)$$

and Z_t is a normalization factor to have $\mathrm{tr}\,\rho_t = 1$.

According to Eq. (10), the average of any observable (O) should be calculated by

$$\langle O\rangle = \mathrm{tr}\,O\rho_t. \quad (13)$$

B. Periodicity constraints

The degree of periodicity of a small part of an infinite system may be classified hierarchically. The zeroth order approximation corresponds to the consistency of the average values of all the boundary and cluster spins. This may be expressed by means of the following system of nonlinear equations:

$$\sum = \langle\sigma^c_1\rangle = \langle\sigma^c_2\rangle = \cdots = \langle\sigma^c_n\rangle = \langle\sigma^b_1\rangle = \langle\sigma^b_2\rangle = \cdots = \langle\sigma^b_m\rangle,$$

where n and m are the number of spins in the cluster and in the boundary, respectively.

Fluctuations of all the spins must be also equal, but in the case of the Ising model we have $\langle\sigma^2\rangle = 1$ and this requirement is automatically satisfied.

The first order approximation should be related to the correlations between nearest neighbors:

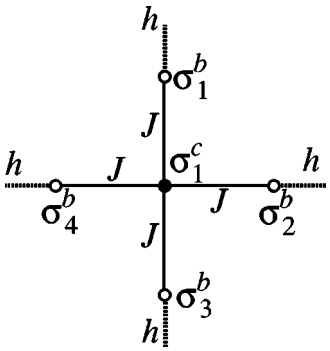

FIG. 2. Schematic representation of the trial model for a single spin cluster. It is equivalent to the Bethe approximation.

$$G^{(1)} = \langle \sigma_i^c \sigma_j^c \rangle = \langle \sigma_i^b \sigma_j^b \rangle = \langle \sigma_i^c \sigma_j^b \rangle$$

for all nearest-neighbor pairs.

This procedure can be generalized to any distance within the boundary-cluster system $(G^{(2)}, G^{(3)}, \ldots)$ [31] until the achievement of the desired level of accuracy. The number of independent equations above depends on the specific structure and symmetry of the cluster, and on the parametrization of the trial Hamiltonian. We have adopted the following practical procedure: once the degree of approximation is decided, new interaction parameters have been added one by one to the trial Hamiltonian until the system of nonlinear consistency equations is satisfied.

III. APPLICATION TO THE SQUARE LATTICE

Three different clusters have been studied: one single spin, two neighbor spins, and a square cluster of four spins.

A. Single spin cluster

For the single spin case (Fig. 2), the four boundary spins are symmetry equivalent. All the correlation functions between spins at the same distances are equal by symmetry, and the periodicity condition can only be applied to the mean values of the central and surrounding spins ($\langle \sigma^c \rangle = \langle \sigma^b \rangle$). As there are no first neighbors among the boundary spins, the trial Hamiltonian may be expressed in terms of a single external field:

$$H_t = H_0 + \Delta H_0 = -(J\sigma_1^c + h)\sum_{i=1}^{4} \sigma_i^b.$$

Thus there is a single nonlinear equation in terms of a single parameter (h), and the method leads to the Bethe approximation [6].

B. Two spin cluster

For the two spin cluster (Fig. 3) both spins in the cluster are symmetry equivalent ($\Sigma_1 = \langle \sigma_1^c \rangle = \langle \sigma_2^c \rangle$) and among the six boundary spins two classes may be distinguished:

$$\sum\nolimits_2 = \langle \sigma_1^b \rangle = \langle \sigma_2^b \rangle = \langle \sigma_4^b \rangle = \langle \sigma_5^b \rangle,$$

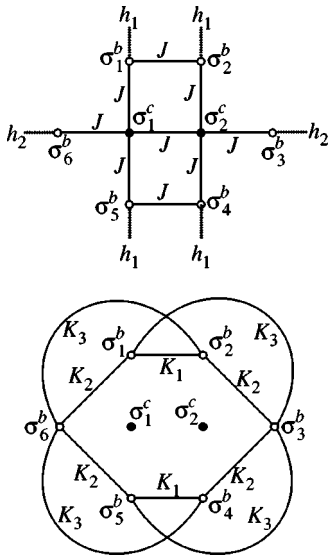

FIG. 3. Approximations for the two spin cluster. Top: couplings and external fields for the zeroth order approximation. Two independent effective fields (h_1 and h_2) are needed. Bottom: first order approximation; three couplings (K_1, K_2, and K_3) are included to make the correlations between first neighbors consistent. The same model is valid to extend the periodicity up to third order.

$$\sum\nolimits_3 = \langle \sigma_3^b \rangle = \langle \sigma_6^b \rangle.$$

The periodicity condition in zeroth order leads to

$$\sum\nolimits_1 = \sum\nolimits_2 = \sum\nolimits_3. \tag{14}$$

The simplest trial Hamiltonian to express the probability density of the boundary spins is

$$H_t = H_0 + \Delta H_0$$

with

$$H_0 = -J[\sigma_1^c \sigma_2^c + \sigma_1^b \sigma_2^b + \sigma_4^b \sigma_5^b + \sigma_1^c(\sigma_1^b + \sigma_5^b + \sigma_6^b) + \sigma_2^c(\sigma_2^b + \sigma_3^b + \sigma_4^b)]$$

and

$$\Delta H_0 = -h_1(\sigma_1^b + \sigma_2^b + \sigma_4^b + \sigma_5^b) - h_2(\sigma_3^b + \sigma_6^b).$$

The two effective fields h_1 and h_2 must be obtained to solve the system of Eq. (14) (two independent nonlinear equations in terms of two effective unknown fields).

One can improve the periodicity of the system by taking into account the correlations between nearest neighbors. According to Fig. 3 these correlations may be grouped into four symmetry independent sets:

$$G_1^{(1)} = \langle \sigma_1^c \sigma_2^c \rangle,$$

$$G_2^{(1)} = \langle \sigma_1^b \sigma_2^b \rangle = \langle \sigma_4^b \sigma_5^b \rangle,$$

$$G_3^{(1)} = \langle \sigma_1^c \sigma_6^b \rangle = \langle \sigma_2^c \sigma_3^b \rangle,$$

$$G_4^{(1)} = \langle \sigma_1^c \sigma_1^b \rangle = \langle \sigma_1^c \sigma_5^b \rangle = \langle \sigma_2^c \sigma_2^b \rangle = \langle \sigma_2^c \sigma_4^b \rangle.$$

Thus the three new consistency equations needed to obtain the first order approximation are

$$G_1^{(1)} = G_2^{(1)} = G_3^{(1)} = G_4^{(1)}. \tag{15}$$

These three new equations are not independent of the relations in Eq. (14); the solutions for the zeroth order approximation also give $G_2^{(1)} = G_4^{(1)}$. However, the simultaneous accomplishment of Eqs. (14) and (15) (five nonlinear equations) requires the inclusion of three quadratic couplings (Fig. 3), and the following terms have to be added to the trial Hamiltonian:

$$\Delta H_1 = -K_1(\sigma_1^b \sigma_2^b + \sigma_4^b \sigma_5^b) - K_2[\sigma_3^b(\sigma_2^b + \sigma_4^b) + \sigma_6^b(\sigma_1^b + \sigma_5^b)] - K_3[\sigma_3^b(\sigma_1^b + \sigma_4^b) + \sigma_6^b(\sigma_2^b + \sigma_4^b)].$$

K_1 adds an extra contribution to J, and K_2 and K_3 increase the correlation between second and third neighbors in the boundary.

The next approximation order may be achieved by taking into account the correlations between second neighbors, that can be grouped according to symmetry as

$$G_1^{(2)} = \langle \sigma_1^c \sigma_2^b \rangle = \langle \sigma_1^c \sigma_4^b \rangle = \langle \sigma_2^c \sigma_1^b \rangle = \langle \sigma_2^c \sigma_5^b \rangle,$$

$$G_2^{(2)} = \langle \sigma_6^b \sigma_1^b \rangle = \langle \sigma_2^b \sigma_3^b \rangle = \langle \sigma_3^b \sigma_4^b \rangle = \langle \sigma_5^b \sigma_6^b \rangle.$$

But the new relation ($G_1^{(2)} = G_2^{(2)}$) necessary to extend the periodicity to this level is not independent and it is already fulfilled by the solutions of the first order approximation [Eqs. (14) and (15)]. The same remark applies to the correlations between third neighbors. The consistency equations are not independent, and for the same trial Hamiltonian the following relation is satisfied:

$$G_1^{(3)} = G_2^{(3)},$$

where the two symmetry independent correlations are

$$G_1^{(3)} = \langle \sigma_1^c \sigma_3^b \rangle = \langle \sigma_2^c \sigma_6^b \rangle,$$

$$G_2^{(3)} = \langle \sigma_1^b \sigma_5^b \rangle = \langle \sigma_2^b \sigma_4^b \rangle.$$

Therefore the trial Hamiltonian $H_t = H_0 + \Delta H_0 + \Delta H_1$ also corresponds to the third order approximation, that is, the periodicity extends up to the correlations between third neighbors. The rest of pair and n-body correlation functions do not satisfy their corresponding consistency equations.

C. Four spin cluster

The eight boundary spins are equivalent by symmetry (Fig. 4), and the only condition about the average values of all the spins is $\Sigma = \langle \sigma^c \rangle = \langle \sigma^b \rangle$. The simplest trial Hamiltonian contains a single external field:

$$H_t = H_0 + \Delta H_0 = H_0 - h \sum_{i=1}^{8} \sigma_i^b.$$

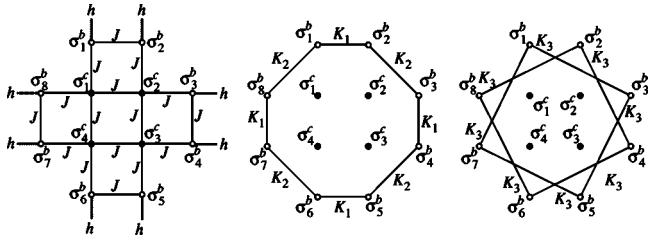

FIG. 4. The square cluster. Left: couplings and external fields for the zeroth order approximation. Middle: first order approximation; correlations between first neighbors are equal. Right: necessary couplings to extend the periodicity to second neighbors.

The first order approximation includes correlations between first neighbors that may be grouped into three symmetry independent sets

$$G_1^{(1)} = \langle \sigma_1^c \sigma_2^c \rangle = \langle \sigma_2^c \sigma_3^c \rangle = \langle \sigma_3^c \sigma_4^c \rangle = \langle \sigma_4^c \sigma_1^c \rangle,$$

$$G_2^{(1)} = \langle \sigma_1^c \sigma_1^b \rangle = \langle \sigma_1^c \sigma_8^b \rangle = \langle \sigma_2^c \sigma_2^b \rangle = \langle \sigma_2^c \sigma_3^b \rangle = \langle \sigma_3^c \sigma_4^b \rangle = \langle \sigma_3^c \sigma_5^b \rangle = \langle \sigma_4^c \sigma_6^b \rangle = \langle \sigma_4^c \sigma_7^b \rangle,$$

$$G_3^{(1)} = \langle \sigma_1^b \sigma_2^b \rangle = \langle \sigma_3^b \sigma_4^b \rangle = \langle \sigma_5^b \sigma_6^b \rangle = \langle \sigma_7^b \sigma_8^b \rangle$$

and the consistency equations for the correlations are

$$G_1^{(1)} = G_2^{(1)} = G_3^{(1)}.$$

The trial Hamiltonian for the boundary spins is $H_t = H_0 + \Delta H_0 + \Delta H_1$, where the new contribution is (Fig. 4)

$$\Delta H_1 = -K_1(\sigma_1^b \sigma_2^b + \sigma_3^b \sigma_4^b + \sigma_5^b \sigma_6^b + \sigma_7^b \sigma_8^b) - K_2(\sigma_8^b \sigma_1^b + \sigma_2^b \sigma_3^b + \sigma_4^b \sigma_5^b + \sigma_6^b \sigma_7^b).$$

Up to this degree of approximation, a system of three nonlinear equations must be solved in terms of h, K_1, and K_2.

Correlations between second neighbors may be grouped into three classes:

$$G_1^{(2)} = \langle \sigma_1^c \sigma_3^c \rangle = \langle \sigma_2^c \sigma_4^c \rangle,$$

$$G_2^{(2)} = \langle \sigma_1^c \sigma_2^b \rangle = \langle \sigma_1^c \sigma_7^b \rangle = \langle \sigma_2^c \sigma_1^b \rangle = \langle \sigma_2^c \sigma_4^b \rangle = \langle \sigma_3^c \sigma_3^b \rangle = \langle \sigma_3^c \sigma_6^b \rangle = \langle \sigma_4^c \sigma_5^b \rangle = \langle \sigma_4^c \sigma_8^b \rangle,$$

$$G_3^{(2)} = \langle \sigma_8^b \sigma_1^b \rangle = \langle \sigma_2^b \sigma_3^b \rangle = \langle \sigma_4^b \sigma_5^b \rangle = \langle \sigma_6^b \sigma_7^b \rangle$$

giving two more equations:

$$G_1^{(2)} = G_2^{(2)} = G_3^{(2)}.$$

Nevertheless, all the equations are not independent and it is enough to add a single coupling to extend the periodicity of correlations to second neighbors (Fig. 4):

$$\Delta H_2 = -K_3(\sigma_1^b \sigma_3^b + \sigma_2^b \sigma_4^b + \sigma_3^b \sigma_5^b + \sigma_4^b \sigma_6^b + \sigma_5^b \sigma_7^b + \sigma_6^b \sigma_8^b + \sigma_7^b \sigma_1^b + \sigma_8^b \sigma_2^b).$$

IV. RESULTS AND DISCUSSION

Once the order of the approximation and model couplings have been chosen, the nonlinear equations can be solved by

TABLE I. Results for different models and approximations. N is the number of spins involved in the calculation of the trace. M is the number of nonlinear equations involved. k_BT_c/J is the transition temperature. $G_c^{(1)}(T_c)$ and $G_c^{(2)}(T_c)$ are the values of the connected correlation functions between first and second neighbors, respectively, at the transition point.

Model	N	Approx.	M	k_BT_c/J	$G_c^{(1)}(T_c)$	$G_c^{(2)}(T_c)$
Mean field	1		1	4.000		
Single spin[a]	5	0	1	2.885	0.333	0.111
Two spin	8	0	2	2.770	0.380[b]	0.191[b]
		1–3	5	2.418	0.563	0.445
Four spin	12	0	1	2.831	0.274[b]	0.138[b]
		1	3	2.428	0.559	0.439[b]
		2	4	2.351	0.607	0.501
Exact[c]				2.269	0.707	0.637

[a]It is equivalent to the Bethe approximation.
[b]As the periodicity requirements do not force the consistency of these correlation functions, the average values are shown.
[c]From Refs. [27,29].

any standard numerical technique. A summary of the results appears in Table I: transition temperatures and values of the connected correlation functions ($G_c^{(1,2)}=\langle\sigma^2\rangle-\langle\sigma\rangle^2$) between first and second neighbors at the critical temperature. Although the present method does not contain the mean-field approximation as a particular case, its transition temperature is cited for comparison. The computational effort for each case is related with two magnitudes. On the one hand the calculation of the statistical averages [Eq. (13)] depends on the total number of spins (N) needed to describe a statistical configuration, that is, the size of the cluster. On the other hand, the number of independent nonlinear equations to be solved (M) increases as the degree of periodicity is improved, or the symmetry of the cluster is lowered. The number of iterations needed to solve M nonlinear equations depends on the behavior of the functions, the required accuracy, and the starting point. In the present calculations, about 10–20 iterations were enough, and in each iteration the equations are evaluated $M+1$ times. For each evaluation $M+2$ statistical sums over all the spins must be done: one for the partition function, and $M+1$ for the traces of Eq. (13). As the number of terms added up in the traces is 2^N for Ising spins, the time needed to perform a calculation at a given temperature is proportional to $10(M+1)(M+2)2^N$. Thus the system size is the magnitude that mainly limits the complexity of the calculations. For instance, the typical computer time needed to perform a single temperature calculation for the case $M=4$ and $N=12$ in a 466-MHz Compaq Alpha EV6 workstation is about several seconds.

The influence of the consistency of the correlations is remarkable. For instance, in the case of the four spin cluster, the error in the transition temperature goes down from 25% in the zeroth-order case to 7% in the first order approximation, and the heights of the peaks in the connected correlation functions show a similar behavior. The obtained transition temperatures in Table I, particularly the best result of $k_BT_c/J=2.351$ for the four spin cluster, can be compared with the results of some of the approximation methods proposed in the literature. The effective-field method with correlations of Taggart [17], double-chain approximation [20], modified effective-field approach [18], and expanded Bethe-Peierls approximation [19] give $k_BT_c/J=2.680$, 2.500, 2.576, and 2.486, respectively. The result of Galam [7] is exceptionally accurate: $k_BT_c/J=2.273$. Unfortunately, the application of the method proposed in Ref. [7] seems to be restricted to spin systems, and there is no obvious way to establish a hierarchical approximation scheme. The cluster-variation method in the Tanoji [24,25] approximation, where 44 variational parameters are needed, gives $k_BT_c/J=2.346$, comparable with our result. The transition temperature in mean-field approximation, applying self-consistency to the central spins of a cluster of 181 spins is $k_BT_c/J=2.360$ [8]. Also, the best transition temperature of the multi-effective-field theory (16 spins and 5 effective fields) is $k_BT_c/J=2.357$ [26]. Our slightly better result using a smaller cluster might be related to a more accurate treatment of the periodicity.

Figure 5 shows the dependence on temperature of the order-parameter and connected correlation functions between first neighbors for the Onsager's exact solution, Bethe approximation, and the three studied cases of the four spin cluster. The difference between the Bethe approximation and zeroth order approximation of the four spin cluster is just the number of spins involved in the calculation. The effect of increasing the size of the cluster is much less important than the improvement obtained by taking the periodicity of the correlations into account (compare the curves corresponding to the Bethe, zeroth, and first order approximation). The comparison between the results of the two and four spin clusters is not so direct. If we consider the zeroth approximation for the two and four spin clusters the transition temperatures and correlation functions for the smaller cluster are better. The reason for this apparent inconsistency is related to the symmetry of the cluster. As the two spin cluster is less symmetric, two effective fields are necessary to make all the mean values of the spins equal, while in one and four spin clusters one model parameter is enough. Thus it can be inferred that, within a given symmetry, as the consistency of

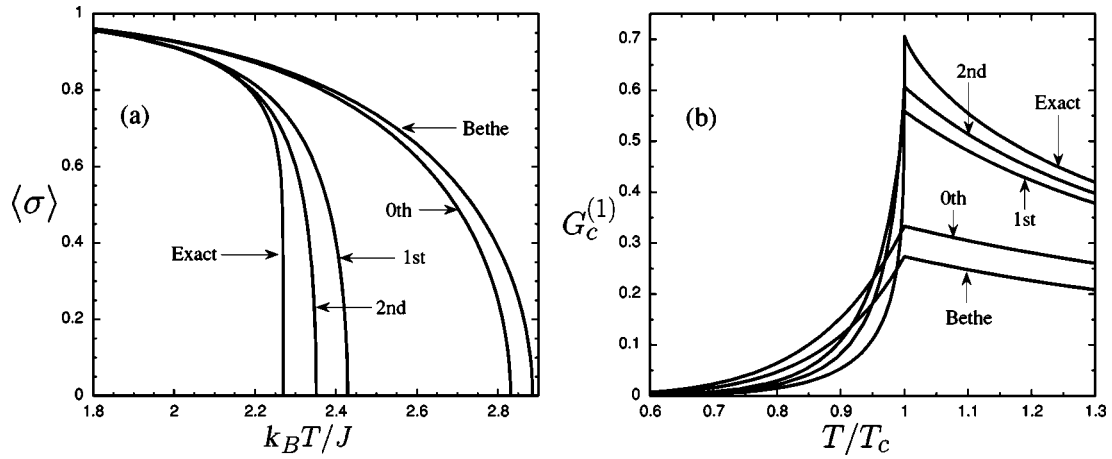

FIG. 5. Results of the four spin cluster in zeroth, first, and second order approximations together with the Bethe approximation and Onsager's exact solution. Evolution with temperature of the (a) order-parameter and (b) connected correlation functions between first neighbors.

periodicity is improved, the evolution of the magnetization tends to the exact values. In all the cases the magnetization shows mean-field critical exponents; an analysis of the coherent anomaly, as in Ref. [8], could give a proper estimation of the ability of the method to be used in the extrapolation of nonclassical critical exponents. Although in this work the method has been used to study a simple test system, the universality of its foundations and the results obtained are encouraging to test its application in more sophisticated Hamiltonian models.

ACKNOWLEDGMENTS

This work was supported by the Spanish Ministry of Science and Technology (Project No. MAT 2002-00086) and the University of The Basque Country (Project No. 00063.310-13564).

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