Importance of multispin couplings in renormalized Hamiltonians

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We introduce a Monte Carlo approach to the calculation of more distant renormalized interactions with higher accuracy than is possible with previous methods. We have applied our method to study the effects of multispin interactions, which turn out to be far more important than commonly assumed. Even though the individual multispin interactions usually have smaller coupling constants than two-spin interactions, they can dominate the effects of two-spin interactions because they are so numerous.

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I. INTRODUCTION

The Monte Carlo (MC) renormalization group [1] simulations have been used extensively in the study of critical phenomena. Each such investigation generally approximates the renormalized Hamiltonian with only a finite number of coupling constants. For applications to the two- and three-dimensional Ising model, this number has increased considerably with time, from 3 in 1979 [2] to 99 in 1992 [3]. A proposed criterion for ordering the couplings according to their importance was introduced by Blöte *et al*. [4] As a general rule, it is believed that couplings tend to become less important when they involve more spins and when the spins are more distant of each other. It is just this assumption that we investigate in this paper, with the conclusion that multispin couplings are far more important than usually believed.

Several methods have been created for the purpose of calculating the coupling constants of the renormalized system [5–7]. Recently we have developed a different approach that enables the calculation of more interactions with higher accuracy than the earlier methods. [8] Our method is based on the Brandt-Ron (BR) representation [9] of renormalization group transformation, which yields useful information that was not available before. An important contribution of this calculation is that it provides a stable method for calculating *all* couplings that fit within a prechosen distance. This feature is the basis of the present work. In fact, we are able to use the BR representation to obtain previously unavailable information about the importance of more distant multispin coupling constants, without the necessity of calculating them individually.

The most similar calculation to ours that we have found in the literature was carried out by Callaway and Petronizio [7] in 1984. They showed how to extract individual coupling constants in a related manner, but suffered from the difficulty that the isolation of a particular coupling constant is not unique and different calculations result with different values. The only consistent way to deal with the problem is to take *all* possibilities into account at each level of approximation, as been done in Ref. [9].

In this paper, we are showing how we can learn something about the relationship between two-spin and multispin couplings without necessarily calculating the values of any *particular* coupling constants.

In the following section the Brandt-Ron representation is reviewed. Its use in determining coupling constants is briefly described in Sec. III. The method for an indirect estimation of coupling constants is introduced in Sec. IV. Results for the two- and three-dimensional Ising models are presented in Secs. V and VI.

II. THE BRANDT-RON REPRESENTATION

The Brandt-Ron representation was introduced in Ref. [9] and used for the calculation of coupling constants of renormalized systems in Ref. [8]. This representation is based on the following central idea. The interactions between spins are described by the conditional probability of a specific spin to be $+1$ given explicit values of a set of its neighboring spins. This set of spins and their values is called a ''neighborhood.'' Let m be the number of spins in the neighborhood under consideration, then P_+^m is the *table* of the conditional probabilities of all possible assignment of the spins in that particular neighborhood. From a Monte Carlo simulation on a given lattice, a sequence of renormalized (block spin) configurations is generated, using the majority-rule transformation on 2×2 blocks, from which the P_+ table is measured. It has been shown in Ref. [9], for the $d=2$ Ising model using the majority-rule transformation on 2×2 blocks, that it is only important to achieve equilibrium at the local scale of the neighborhood's size.

Similar results were later obtained also for the $d=3$ case. In addition, the method can be used equally well with any other RG transformation as was demonstrated in Ref. [10].

For the $d=2$ Ising model Brandt and Ron have used their representation in a sophisticated algorithm that constructed an appropriate set of growing neighborhoods, based on the amount of statistics accumulated during the course of an MC simulation. In this way they were able to systematically reduce the truncation error involved in the calculation [9].

III. CALCULATION OF COUPLINGS FROM P_+'S

Ron and Swendsen have developed a method based on these P_+ tables for a stable calculation of renormalized

Hamiltonian [8]. The calculation is done systematically for values of m, the number of spins in the neighborhood. We identify *all* possible even interactions that could be placed within that neighborhood with one spin placed at the center. All possible orientations are included, as demanded by translational invariance. The P_+ table is then calculated for every possible arrangement of the m spins. Naturally, the symmetries of the model are taken into account to reduce the number of entries in the table. Finally, each entry j of the P_+ table, P_j, is translated into its equivalent effective field

$$\mathcal{H}_j = -(1/2)\ln[(1-P_j)/P_j]. \quad (1)$$

The determination of the renormalized couplings follows by minimizing the sum (over j) of weighted deviations of the Hamiltonian from the value of the $\mathcal{H}_j$ obtained from the P_j by Eq. 1. This approach allows the computation of more interactions with higher accuracy than previous methods.

Still, it is clear that as m is increased, the number and complexity of the possible interactions grow rapidly, and the size of the P_+ tables can quickly become intractable. It was this observation that has led us to adopt a different approach to allow us to obtain additional information on the strength and importance of distant and/or multispin interactions without going through the full procedure of computing every coupling.

IV. FIXED NEIGHBORHOOD COMPUTATION OF P_+'S

The calculation of the P_+ tables as carried out by Brandt and Ron used a normal Monte Carlo simulation of the spin system. This means that each neighborhood appears with a fixed frequency that reflects its probability of appearance in the canonical distribution. Since the accuracy of each P_+ strongly depends on how many samples contribute, rare neighborhoods necessarily give very poorly approximated P_+ values.

To deal with this problem, we have developed a method that enables an accurate calculation of the P_+ value of *any* neighborhood of interest, independent of its thermal probability. This is achieved as follows.

Denote by N_m a particular neighborhood consisting of m spins around the central spin. On a slightly larger lattice, fix the m spins to equal N_m, leaving the central spin and the spins around that neighborhood undetermined. This is the given coarse (block spin) system. The corresponding fine system of spins is defined on a doubled linear size lattice, such that each fixed block spin is replaced, for example, by a 2^d block of spins of the same sign, where d is the dimension of the system. The 2^d central spins and all those surrounding the neighborhood may initially assume any value. The initial fine configuration is thus *consistent* with N_m.

An MC simulation of the fine system is performed with the constraint that configurations are restricted to those that are compatible with N_m. The restriction is actually posed only on those fine spins which belong upon the renormalization transformation to the m spins in N_m. That is, if a proposed spin flip would violate the condition that the majority of spins in a block has the same sign as the renormalized spin in N_m, it is rejected. If the spin flip would result in a block with an equal number of positive and negative spins, the acceptance probability of the move is 0.5. Brandt and Ron called a similar process in which the *entire* renormalized system is fixed "compatible Monte Carlo" (CMC) [9] and showed that the procedure has a very small correlation time, independent of the lattice size, because of the local nature of the relaxation, even though the system is at criticality. Since the demand here is compatibility only with N_m, it will be referred to as the *partial* CMC. Observe that the generated configurations are free to assume all possible combinations of $+1$'s and -1's at the central block of spins. Thus, the P_+ value of N_m can be easily calculated to a desired accuracy by counting the number of $+1$'s and -1's appearing at the center of N_m throughout the simulation.

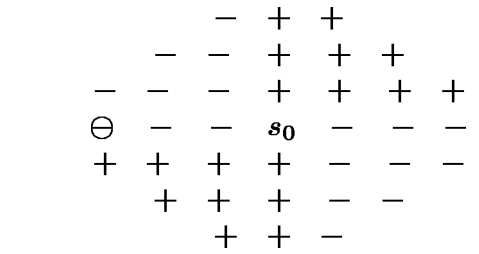

FIG. 1. The 36-spin neighborhood surrounding a spin s_0, denoted by $A(-)$. $A(+)$ is obtained by flipping the -1 marked by a ○.

V. TWO-DIMENSIONAL ISING MODEL

As a first application of the fixed-neighborhood method to calculate particular P_+ values, we have investigated the interactions between two spins that are three lattice constants apart for the two-dimensional Ising model at criticality.

Denote by $A(-)$ the neighborhood in Fig. 1. Since half of its $m=36$ spins are up and half down, all arranged in a symmetric order around the center s_0, its P_+ value is exactly .5, i.e., $P_+[A(-)]=0.5$. Flipping the spin s_3 marked by ○ would break that symmetry. To measure the P_+ value for this neighborhood, denoted by $A(+)$, we have placed it on a 9^2 lattice and performed 5×10^9 partial CMC sweeps on the corresponding fine spin level of size 18^2 with periodic boundary conditions. We obtained $P_+[A(+)] = 0.500\,388\,7(83)$. This is in line with normal expectations in a ferromagnetic model, since an additional positive spin increased the probability that the central spin was positive.

Now consider the neighborhood in Fig. 2, denoted by $B(-)$, and the corresponding neighborhood $B(+)$, in which the circled spin is changed to a positive value. Unexpectedly, the flipped spin had a *qualitatively* different effect. The measured values were $P_+[B(-)]=0.939\,413\,7(32)$ and $P_+[B(+)]=0.939\,397\,2(28)$. So that $P_+[B(+)]$ turned out to be *smaller* than $P_+[B(-)]$. This is somewhat counter intuitive, since an additional positive spin in its neighborhood *reduced* the probability that the central spin was positive.

The difference, of course, reflects the effects of the multispin couplings in the renormalized Hamiltonians.

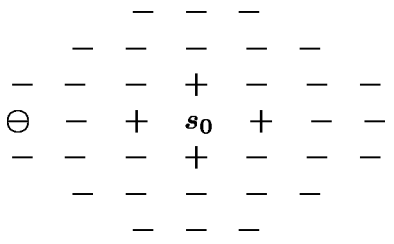

FIG. 2. The 36-spin neighborhood surrounding a spin s_0, denoted by $B(-)$. $B(+)$ is obtained by flipping the -1 marked by a ○.

On one hand the P_+ values can be translated into corresponding effective fields on the central spin using Eq. 1: $\mathcal{H}[A(-)]=0$, $\mathcal{H}[A(+)]=0.000\,777\,4$, $\mathcal{H}[B(-)]=1.370\,558$, and $\mathcal{H}(B(+))=1.370\,439$. On the other hand the Hamiltonian is usually written in the form

$$\mathcal{H}=\sum_i K_i S_i, \tag{2}$$

where the K_i's are the coupling constants and the S_i's are various sums of products of spins. The differences $\delta\mathcal{H}(A)=\mathcal{H}[A(+)]-\mathcal{H}[A(-)]$ and $\delta\mathcal{H}(B)=\mathcal{H}[B(+)]-\mathcal{H}[B(-)]$ would only depend on couplings involving the central spin and the flipped spin s_3, so that

$$0.000\,777\,4=\delta\mathcal{H}(A)=2\left[K_3+\sum_\alpha K_\alpha s_i^A s_j^A + \text{higher-order terms}\right] \tag{3}$$

$$-0.000\,119=\delta\mathcal{H}(B)=2\left[K_3+\sum_\alpha K_\alpha s_i^B s_j^B + \text{higher-order terms}\right], \tag{4}$$

where K_3 is the coupling constant of the two-spin coupling of distance three lattice constants, the K_α's are all the four-spin couplings that fit in the neighborhood, while s_i^A (s_i^B) and s_j^A (s_j^B) are spins in the neighborhood $A(-)$ [$B(-)$] other than s_3. Since the K_3 term is identical in Eqs. 3 and (4), the difference must come from the multispin terms. That is, even if K_3 is larger than every one of the multispin-spin coupling constants, it must be *smaller* than their *sum*. In other words, we may conclude that the two-spin coupling does not dominate the Hamiltonian in this case, but that the sum of the contributions of the multispin couplings is more important.

This result can even be seen for two-spin correlations at shorter distances. For example, from the set of 21 couplings calculated from the P_+^{20} table in Ref. [8], we find that the two-spin coupling of distance 2 is -0.0087. There are 14 multispin couplings within this set that involve these two spins. Consider the neighborhood of 20 positive spins and the one in which a spin two lattice constants from the center is flipped. The contribution of all multispin couplings sums up to 0.010 03, so that the net influence is only 0.001 303. This is significantly smaller, and its sign is opposite to that of the two-spin coupling constant.

Similarly for a spin two lattice constants over and one up, at a distance $\sqrt{5}$. The two-spin coupling is $-0.005\,993$ and the sum of all other couplings is 0.006 258. These again largely cancel out each other with a net influence of 0.000 265.

This near cancellation does not happen for the nearest neighbors or for the next nearest neighbors. In fact, the two-spin coupling of the nearest neighbors is about as eight times as stronger than all relevant multispin couplings, with both having the same sign. The next-nearest-neighbor coupling is only larger by a factor of about three but still has the same sign, while for more distant two-spin couplings, we have observed a change of sign and near cancellation.

It should be pointed out that we also found some limits to the extent of the effects of multispin interactions. For example, we considered a series of neighborhoods generated form $B(-)$ (see Fig. 2) in which all the neighbors, similar to the one marked by ○, at a distance of three lattices constants from the central spin are flipped. The P_+'s for zero through all four of these spins being positive were: 0.939 413 7(32), 0.939 397 2(28), 0.939 375 0(32), 0.939 360 6(46), and 0.939 344 0(44), which made the corresponding differences: 0.000 016 5(43), 0.000 022 2(43), 0.000 014 4(56), and 0.000 016 6(64). Since these differences were nearly the same within the statistical errors, there is no evidence for the influence of significant multispin interactions in this case. The fact that these P_+'s keep on decreasing as more positive spins are introduced, can possibly be explained if one remembers that each spin is actually a block spin that represents the majority of its corresponding fine spins. Introducing a positive block spin among negative ones would result in attracting possible positive spins in its neighborhood, pushing the negative ones away. Thus, the introduced positive block spins have increased the probability of finding more negative spins close to s_0.

VI. THREE-DIMENSIONAL ISING MODEL

For the three-dimensional model, consider a neighborhood of 26 spins that form a $3\times3\times3$ cube around its center. For the neighborhood of all positive spins we obtained $P_+(26+)=0.943\,021\,8(95)$. By flipping one of the corner spins we get $P_+(25+;1-)=0.941\,228\,8(75)$. This probability is lower, as expected from decreasing the number of positive neighbors.

Now consider the neighborhood formed by setting the bottom nine spins of the cube to $+1$, the top nine to -1 and assigning $+1$ to four of the eight spins in the middle layer in a consecutive manner, $P_+(13+;13-)=0.5$. Flipping the positive corner that has more positive neighbors than the others, we find that $P_+(12+;14-)=0.501\,723\,9$. As in two dimensions, we again find a case in which making a spin negative can have a positive effect instead of the more intuitively plausible positive effect. This shows that the strange results found in two dimensions are also found in three dimensions, so they should be regarded as a common feature

of renormalization group transformations.

Again we checked on whether we would find linear behavior for a sequence of spin reversals at a given distance. Because of the greater difficulty in obtaining good statistics in three dimensions, we looked at the third neighbors (located at the corners of the cube). We considered the sequence of all spins positive, one corner reversed, two spins on opposite corners reversed, and three spins, including two opposite corners. The results were: $P_+(26+)=0.943\,021\,8(95)$, $P_+(25+;1-)=0.941\,228\,8(75)$, $P_+(24+;2-)=0.939\,430\,1(131)$, and $P_+(23+;3-)=0.937\,895\,1(165)$, with corresponding differences of $0.001\,79(1)$, $0.001\,80(2)$, and $0.001\,54(2)$. Here, the two opposite spins have independent influences, indicating no detectable multispin effects. However, the third corner spin has an effect that is significantly reduced. We believe that this reflects the fact that it is closer to the previous two spins than the two opposite corners are to each other. Therefore, this example has given us a hint of where the boundary is between needing to include multispin effects, and being able to ignore them.

VII. CONCLUSIONS

In this paper, we have introduced a different method of investigating more distant renormalized interactions with high accuracy. Our studies have indicated that multispin interactions are far more important than commonly assumed. Even though the individual multispin interactions usually have smaller coupling constants than two-spin interactions, the fact that they are very numerous can lead to multispin interactions dominating the effects of two-spin interactions.

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