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Application of the Monte Carlo Method for Evaluating the Niemeijer-van Leeuwen Cumulant Expansion

Z. Rácz and P. Ruján
Institute for Theoretical Physics, Eötvös University, Budapest, Hungary

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We show that the large cell size problem of the real space renormalization can be handled effectively by Monte Carlo methods. As a demonstration, the second-order cumulant expansion is calculated for the three-dimensional simple cubic Ising model, using a $3 \times 3 \times 3$ cell.

I. Introduction

In recent years a variety of methods have been introduced for carrying out renormalization-group transformations [1–5]. Among them the Niemeijer-van Leeuwen cumulant-expansion method [2] is the simplest – both conceptually and technically. It has been applied to several two and three dimensional models [6–14] and the results are surprisingly good. In most cases the critical points and indices, calculated from the second-order cumulant expansion, agree with the available exact and series results within a few percents.

The Niemeijer-van Leeuwen method is a truncation scheme: the expansion goes in powers of the nearest-neighbour coupling, and to a given order only a certain number of couplings are treated self-consistently. In order to have some confidence in the method, one has to investigate the nature of the expansion. Third-order results [15] seem to indicate that the expansion is asymptotic and there is an optimal cell size in every order of the expansion. The investigation of cell-size dependence is not easy [7, 14, 16] since working with cells of n spins means calculation of sums over 2^{n-1} states, which makes the calculation impractical for large n.

Besides the investigation of the cell-size dependence, the problem of large cell-size arises also when applying the Niemeijer-van Leeuwen method to various three-dimensional models.

An obvious candidate to overcome the computational difficulties is the Monte Carlo (MC) method [17, 18]. The idea of combining the renormalization-group and the MC methods has been used first by Ma [5]. He showed that one can derive a renormalization-group transformation by monitoring the time development of the system and by making local measurements i.e. by observing the behaviour of a small number of neighbouring spins. In this way he succeded in estimating not only the static but also the dynamic exponents of the kinetic Ising model.

In this paper we pursue a simpler task, namely we suggest to overcome the problem of large cell size in the cumulant expansion by using the Monte Carlo method for evaluating the needed averages. The MC method is an especially practical tool for our purpose, since in not too large a cell the number of spins is much less than in a usual MC calculation ($10^3 - 10^4$ spins), where the aim is to find the properties of an infinite sytem. So in our case the same number of MC steps/spin requires only a small amount of computer time and the results are much more accurate because the MC samples fill the phase space much more densely.

In order to show how the above idea works we calculated the second-order cumulant expansion for the simple cubic Ising model using a cell of 27 spins. With some effort and lots of computer time this case can be treated exactly [14], so by comparing the results we can judge how the MC method performs.

In Section II we introduce the necessary notation by summarising the Niemeijer-van Leeuwen method. The results of the MC calculation and the comparison with the exact data are presented in Section III.

II. Cumulant Expansion Method

The Niemeijer-van Leeuwen treatment of the Ising model is based on the intuitive Kadanoff picture [19]. The lattice of spins ($s_i = \pm 1$) is divided into an isomorphic lattice of cells, each cell containing n spins. The cells are assumed to behave like Ising spins, their spins (s') being determined by the majority rule:

$$s' = \mathrm{sgn}\left(\sum_{i=1}^{n} s_i\right). \tag{1}$$

The original Hamiltonian $\mathscr{H}(s)$ and the cell Hamiltonian $\mathscr{H}'(s')$ are related by

$$\exp[\mathscr{H}'(s')] = \sum_{\{s\}}{}' \exp[\mathscr{H}(s)], \tag{2}$$

where the summation is restricted to configurations $\{s\}$ compatible with the cell configuration $\{s'\}$. Equation (2) determines the renormalization group transformation ($\mathscr{H}(s) \to \mathscr{H}'(s')$) mapping the model on itself with different coupling constants. Since this transformation cannot be carried out exactly, one has to resort to approximations. In the cumulant expansion scheme $\mathscr{H}(s)$ is separated into an intracell ($\mathscr{H}_0(s)$) and intercell ($\mathscr{V}(s)$) part, containing all the intracell and intercell interactions, respectively. Treating the intercell part as a perturbation the expansion for $\mathscr{H}'(s')$ takes the following form:

$$\mathscr{H}'(s') = \ln \sum_{\{s\}}{}' \exp[\mathscr{H}_0(s)] + \langle \mathscr{V} \rangle_0 + \tfrac{1}{2}(\langle \mathscr{V}^2 \rangle_0 - \langle \mathscr{V} \rangle_0^2) + \cdots, \tag{3}$$

where $\langle\ \rangle_0$ denotes the canonical average in the system without the intercell interactions, calculated at a fixed cell configuration $\{s'\}$:

$$\langle \mathscr{A} \rangle_0 = \frac{\sum_{\{s\}}{}' \mathscr{A}(s) \exp[\mathscr{H}_0(s)]}{\sum_{\{s\}}{}' \exp[\mathscr{H}_0(s)]}. \tag{4}$$

One can see from (3) and (4) that apart from the combinatorial factors the calculation of $\mathscr{H}'(s')$ involves the evaluation of canonical averages of spins and spin correlations in an isolated cell at fixed cell spin. It is clear that the problem of large cells is the problem of calculating these quantities.

Evaluating (3) we find a system of nonlinear equations relating the new set of interaction parameters $\mathbf{K}'$ to the old ones $\mathbf{K}$:

$$\mathbf{K}' = \mathbf{R}(\mathbf{K}). \tag{5}$$

There is a further approximation used for evaluating the mapping $\mathbf{K} \to \mathbf{K}' = \mathbf{R}(\mathbf{K})$, namely the nearest-neighbour coupling is assumed to be a small quantity of first order and the order of every other coupling is determined by the order of the cumulant expansion in which it is generated.

In order to find the critical indices, the approximate renormalization group transformation (5) has to be linearized around its stable fixed point $\mathbf{K}^* = \mathbf{R}(\mathbf{K}^*)$:

$$\mathbf{K}' - \mathbf{K}^* = \mathbf{T}(\mathbf{K} - \mathbf{K}^*). \tag{6}$$

The largest eigenvalue λ_T of $\mathbf{T}$ in the subspace of even spin couplings determines the critical index of the correlation length

$$\nu = \frac{\ln l}{\ln \lambda_T}, \tag{7}$$

where l is the ratio of the new and old lattice constants.

If the starting Hamiltonian includes a magnetic field, then $\mathbf{T}$ has a second relevant eigenvalue λ_H, which is related to the magnetic scaling index by

$$\delta = \left[d \frac{\ln l}{\ln \lambda_H} - 1\right]^{-1}. \tag{8}$$

We have carried out the program outlined above for the Ising model on a simple cubic lattice, using as the basic cell a cube of 27 spins. In this case the second order cumulant expansion includes the nearest neighbour (K), second neighbour (L) and fourth neighbour (M) interactions. They satisfy the following set of recursion equations:

$$K' = g_{11} K + g_{12} L + g_{13} M \tag{9}$$

$$L' = g_{21} K^2 + g_{22} L \tag{10}$$

$$M' = g_{31} K^2, \tag{11}$$

where g_{ik} are expressed through single spin averages $\langle s_i \rangle_0$ and two spin correlations $\langle s_i s_j \rangle_0$ in a single cell at a fixed cell spin. The derivation of their expressions is straightforward but the resulting formulae are too lengthy to record here [20]. Up to the second order they all depend only on K.

Once g_{ik} is known, the remaining steps of the renormalization group procedure (6–7) are carried out easily. The exact calculation of g_{ik} is quite a formidable task, since at fixed cell spin a cell of 27 spins has 2^{26} configurations to be summed over. This problem, however, can be attacked effectively by MC methods, as shown in the next section.

III. Monte Carlo Calculation for the 3 × 3 × 3 Cell

The MC method of estimating canonical averages is well known [17, 18]: an ergodic path is generated in

the phase space and the averages are evaluated as sums over a finite sequence of the path. In our case the ergodic path is generated by simulating the time evolution of a kinetic Ising model [21] consisting of 27 spins. The ensemble averages, needed for g_{ik}, are found as time averages and the additional complication of fixed cell spin condition is taken into account by calculating the single spin averages as

$$\langle s_i \rangle_0 = \frac{1}{\tau} \int_0^\tau s_i(t) \operatorname{sgn}[s'(t)]\, dt, \tag{12}$$

where $s'(t)$ is the cell spin at the moment t.

The two spin correlation functions $\langle s_i s_j \rangle_0$ are invariant under cell spin reflection, so for them the fixed cell spin condition can be omitted. This makes it possible to find $\langle s_i s_j \rangle_0$ exactly. A spin decimation [22] is performed which reduces the number of spins to 13, thus making the problem easily solvable by computer.

There are several unsettled questions in connection with the MC method [23]. For example, it is not known how long the time sequence should be in order that the time average would reliably represent the ensemble average. In this respect the MC calculation is more like an experiment: longer and longer time sequences are tried until the results of several independent runs converge.

As an example of our MC results, on Figure 1 we displayed g_{13} as a function of K. The error bars are estimated from the results of four independent runs, using 3000 MC steps/spin in one run. The computer time required for one point is 5 minutes on a CDC 3300 computer. Similar plots can be drawn for all g_{ik}.

In order to have an idea of how accurately the fixed point of the renormalization group transformation is determined, on Figure 2 we plotted the function $g(K)$, which is defined in the following way: we set $L'=L$ and $M'=M$ in Equations (10) and (11) and the expressions for L and M are substituted in (9). Then one arrives at an equation of the form

$$K' = g(K)\, K \tag{13}$$

and the condition $g(K^*)=1$ gives the fixed point value of K in second order. From Figure 2 one can see that K^* is determined with better than 1 % accuracy.

The results for the critical indices are less accurate. Their calculation involves the evaluation of g_{ik} and dg_{ik}/dK at K^*. Since most of the g_{ik}-s are quite steep functions of K, the derivatives introduce an uncertainty of order 10–15 % in some matrix elements of **T**. This large uncertainty, however, does not appear in the largest eigenvalue (λ_T), because of the restriction that all the eigenvalues of **T** have to be real [24]. It turns out that all the eigenvalues of **T** are real only for a narrow region in the allowed range of parameters,

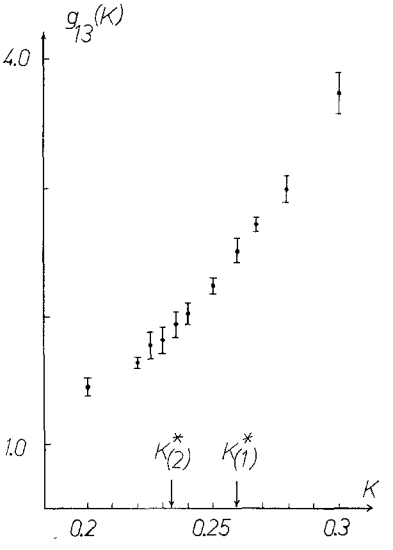

Fig. 1. Monte Carlo results for the function $g_{13}(K)$ defined by Equation (10). The locations of the first and second order fixed points are denoted by K_1^* and K_2^*

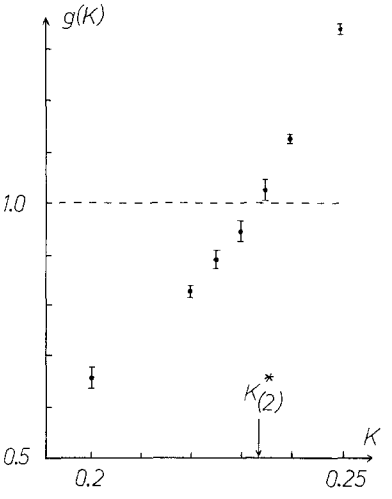

Fig. 2. Monte Carlo results for $g(K)$ defined by Equation (13). From the condition $g(K_2^*)=1$ the second-order fixed point value of K is found to be $K_2^*=0.234\pm0.002$

and in this region the largest eigenvalue is almost constant. This observation severely restricts the possible values of the largest eigenvalue and it brings us back to 5 % accuracy. It is interesting that the largest eigenvalue is quite stable even without the restriction of the reality of the eigenvalues; its uncertainty is less than 10 %.

One can try to avoid the large uncertainty introduced by the numerical derivation of g_{ik}. The derivatives dg_{ik}/dK can be expressed through higher-order (three- and four-point) correlation functions and they can be estimated directly from the MC runs [5]. It turns out,

Table 1. Comparison of the critical parameters obtained by a) Monte Carlo method; b) exact evaluation of the first and second-order cumulant expansion (Hsu and Gunton [14]) and c) high temperature series (Domb [25])

Order of perturbation		K_c	λ_T	λ_H
1st	a)	0.26 ± 0.005	3.6 ± 0.2	16.3 ± 0.4
	b)	0.2599	3.596	16.129
2nd	a)	0.25 ± 0.005	3.6 ± 0.2	–
	b)	0.2371	3.676	14.837
Series	c)	0.2217	5.6	15.6

however, that the MC estimates of the higher-order correlation functions converge much slower than those of the one point functions. In our case (4×3000 MC steps/spin) the accuracy of the direct estimates of dg_{ik}/dK is not better than that of the numerical differentiation. Of course, if the fixed point is known a priori, the direct calculation of dg_{ik}/dK is preferable to the numerical derivation because it requires less computer time.

In Table 1 the results are summarized together with Hsu and Gunton's exact second-order values and with the corresponding high-temperature series estimates [25]. One can see that the MC method performs well, although a little discrepancy remains in the critical point value K_c. Both the linearization of (2) and the direct iteration of the recursion formulae (9, 10, 11) give a somewhat larger value than the exact one. The error introduced by the MC calculation, however, is less, even in this case, than the uncertainty inherent in the second-order cumulant expansion.

In view of the little amount of computer time used for achieving such an accuracy, the method seems to be well suited for more sophisticated calculations. For example the Nienhuis-Nauenberg method [26] could be applied to the three-dimensional Ising model. It would probably give much better results than the second-order cumulant expansion, since this scheme incorporates characteristic three-dimensional interactions, which would enter only in high orders of the cumulant expansion.

A relevant work came to our attention after completing the manuscript. Friedman and Felsteiner [27] used the Monte Carlo technique to carry out renormalization group transformation on finite lattices of two cells with periodic boundary conditions. Their results for the two- and three-dimensional Ising models demonstrate also that the Monte Carlo technique is a practical and accurate method for evaluating renormalization-group transformations.

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Z. Rácz
P. Ruján
Institute for Theoretical Physics
Eötvös University
Budapest, Hungary