Improved cumulant expansion for a renormalization-group treatment of Ising models

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The cumulant expansion of renormalization equations proposed by Niemeijer and van Leeuwen is reexamined, resulting in a considerably improved version of the calculation of the critical properties of Ising systems. In particular the thermal and magnetic eigenvalues are determined to within 0.2 and 1.1%, respectively, of the exact values for the square lattice of spins 1/2, from the second-order calculation in this expansion.

Quite recently Niemeijer and van Leeuwen[1,2] proposed two methods to approximate certain realizations of nonlinear[3] renormalization transformations for Ising systems which avoided the use of continuous spins and the ϵ expansion,[4,5] viz., the cumulant expansion and the cluster expansion. The cluster expansion proved to be more powerful than the cumulant expansion in the particular case of the triangular lattice and resulted in a determination of the critical exponents to within 2% precision (in the worst case) for the seven-cluster approximation. However, the cumulant expansion is an attractive calculational scheme as it is quite simple to apply and provides in principle the basis for a systematic and hopefully convergent determination of critical exponents within the framework of the renormalization group approach to critical phenomena. For these reasons we have attempted to improve the cumulant expansion by enlarging the cell size with the result that by a second-order calculation for the square Ising lattice of spins $\frac{1}{2}$ we have determined the thermal and magnetic eigenvalues to within 0.2% and 1.1% of their exact values, respectively. The calculation is extremely straightforward and simple to perform and can be carried out on a computer in less than 1 sec.

To begin with, we note that the relatively poor convergence of the cumulant expansion for the triangular lattice might be due to the smallness of the basic cell chosen in Ref. 1, where it consists of a triangle of three spins. The fact that the number of intercell versus intracell interactions is two versus three in first order is rather large, suggests that the corresponding choice of the unperturbed Hamiltonian H^0 may be improved, since the coefficients which occur in the resulting renormalization equations carry little information, as they are statistical averages of spin variables using

$$\exp\left(-\beta H^0 / \sum_e e^{-\beta H^0}\right)$$

as the density matrix. Hence one might hope that a better approximation to the renormalization equations can be obtained by choosing a larger cell size, with a correspondingly improved H^0. To test this idea, we considered a square Ising lattice (which is more suitable for our purpose) with square cells containing nine spins (see Fig. 1).

We will follow the notation of Ref. 1 to which the reader is referred for details of our calculation. A brief summary of the procedure is as follows. A cell spin S_i' is associated with each cell, with

$$S_i' = \mathrm{sign}\left(\sum_{n=1}^{9} S_i^n\right), \tag{1}$$

where n numbers the sites in the ith cell. For a given S_i' the site spins $\{S_i^l\}$ can still assume 2^8

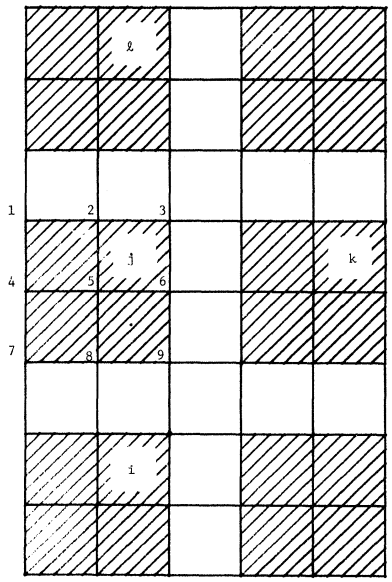

FIG. 1. Cells on the quadratic lattice. The symbols i, j, k, l label typical cells while the numbers 1, 2, ..., 9 label site spins and correspond to the numbering which is used in the text.

configurations σ_i^k, $k = 1, \ldots, 256$. The renormalization equations are defined by performing a partial sum in the exact partition function over all the internal cell variables $\{\sigma\}$ compatible with a given set of cell spin values $\{S'\}$. This generates a new Hamiltonian $H'(\{S'\})$ which describes the interactions between the cell spins and which can be decomposed as

$$H' = \sum_a K'_a S'_a \ , \tag{2}$$

where

$$S_a = \prod_{i \in a} S_i$$

and where a runs over all the subsets of the lattice. This is of the same form as the most general version of the original Hamiltonian, with the cell spin variables replacing the site spins and the cell interaction parameters K'_a replacing the site spin interactions K_a. The renormalization equations are

$$K'_a = K'_a(\{K\}) \ . \tag{3}$$

The transformation (3) should have a nontrivial fixed point K^* at which the linearized transformation

$$\left(\frac{\partial K'_\alpha}{\partial K_\beta}\right)_{K=K^*} = T_{\alpha\beta} \tag{4}$$

should have only two eigenvalue λ_T and λ_H which are greater than unity.[6] These are related to the critical exponents by

$$\alpha = 2 - d \ln l / (\ln \lambda_T) \ \text{ and } \ \sigma = 1/(d \ln l / \ln \lambda_H - 1) \ ,$$

where d is the dimensionality and l is the lattice spacing of the cells measured in units of the site spacing. Since in our case $l = 3$, $d = 2$, and we know that[7] $\alpha = 0$ and[8] $\delta = 15$, we should have $\lambda_T = 3$ and $\lambda_H = 9^{15/16}$. As it is impossible to calculate the renormalization equations as given in Eq. (3) exactly, we must turn to an approximation procedure which we choose as follows. Split the Hamiltonian into an unperturbed part H^0 and a perturbation V:

$$H = H^0 + V \ , \tag{5}$$

where H^0 contains all interactions inside the cells and V all interactions between the cells. We then can write

$$\exp H'(S') = \left(\sum_{\{\sigma\}} \exp H^0(S', \sigma)\right) \langle \exp V \rangle_0 , \tag{6}$$

where

$$\langle \exp V \rangle_0 = \left(\sum_{\{\sigma\}} \exp V(S', \sigma) \exp H^0(S', \sigma)\right) \Big/ \sum_{\{\sigma\}} \exp H^0(S', \sigma) \ . \tag{7}$$

Expression (7) still is exact and can be approximated by evaluating successive terms in the cumulant expansion

$$\langle \exp V \rangle_0 = \exp\left[\langle V \rangle_0 + \tfrac{1}{2}\{\langle V^2 \rangle_0 - \langle V \rangle_0^2\} + \cdots\right] \tag{8}$$

for $\langle \exp V \rangle_0$ (first term is the first approximation, first plus second is the second approximation, etc.). In first order if one starts with only nearest-neighbor interactions of strengths K and magnetic field h, one obtains for the interaction between two nearest-neighbor cells and the renormalized magnetic field h'

$$\langle V_{ij} \rangle_0 = K(\langle S_i^1 \rangle_0 \langle S_j^7 \rangle_0 + \langle S_i^2 \rangle_0 \langle S_j^8 \rangle_0 + \langle S_i^3 \rangle_0 \langle S_j^9 \rangle_0) S'_i S'_j \ , \tag{9}$$

$$h' = \sum_{S'_i, S'_j} S'_i V_{ij} + \tfrac{1}{2} \sum_{S'_i} S'_i \ln Z_0(S'_i) \ , \tag{10}$$

where

$$Z_0(S'_i) = \sum_{\{\sigma_i\}} \exp H_i^0(S'_i, \sigma_i)$$

and H_i^0 is the cell Hamiltonian. The site numbering as well as the cell labeling of Fig. 1 has been used. This leads to a first-order renormalization equation

$$K' = (2\langle S^1 \rangle_0^2 + \langle S^2 \rangle_0^2) K \tag{11}$$

for zero magnetic field. A fixed-point solution of this equation is $K' = K = K^*$ and is found by numerical means to be $K^* = 0.4697$. The eigenvalues of the T matrix, as defined in Eq. (4), were then found from Eq. (11) and Eq. (10) to be $\lambda_T = 2.7689$ and $\lambda_H = 8.4566$.

In second order, one also generates next-nearest-(L') and next-next-nearest-(M') neighbor interactions even if one starts with just nearest-neighbor interactions in the initial Hamiltonian. If we consider the nearest-neighbor coupling K as the first-order quantity, then one sees that L' and M' are second-order terms. Thus to be complete in second order, one must also treat the effect of L and M interactions in H^0 and V. The set of renormalization equations that one then finds for zero magnetic field is

$$\begin{aligned} K' &= \langle V_{ij} \rangle_0 \ , \\ L' &= L \langle S_i^3 \rangle_0 \langle S_k^7 \rangle_0 + 2\langle V_{ij} V_{jk} \rangle_{0c} \ , \\ M' &= \langle V_{ij} V_{jl} \rangle_{0c} \ , \end{aligned} \tag{12}$$

where it is understood that the cell spin dependence on the right-hand side is to be suppressed. The terms $\langle V_{ij} V_{jk} \rangle_{0c}$ and $\langle V_{ij} V_{jl} \rangle_{0c}$ are proportional to K^2 and functions of single-spin and two-spin cell-correlation functions. The explicit form of Eq. (12) is

TABLE I. Eigenvalues and critical temperature for the square lattice.

Approximation	γ_T	λ_H	K_c
First-order perturbation	2.7689	8.4566	0.4697
Second-order perturbation	3.0068	7.9271	0.4302
Exact	3	7.845	0.4407

$$
\begin{aligned}
K' &= K(2f_1^2+f_2^2)+4Lf_1f_2+2M(2f_1f_2+f_2f_3)\,,\\
L' &= Lf_1^2+2K^2[2f_1^2(1+2f_4+f_6-4f_1^2)\\
&\quad +2f_1f_2(f_5+f_7-2f_1f_2)+f_2^2(f_8-f_2^2)]\,,\\
M' &= K^2[2f_1^2(f_4+f_6-2f_1^2)+4f_1f_2(f_5-f_1f_2)\\
&\quad +f_2^2(f_9-f_2^2)]\,,
\end{aligned}
\tag{13}
$$

where

$$
f_1=\langle S^1\rangle_0,\ f_2=\langle S^2\rangle_0,\ f_3=\langle S^5\rangle_0,
$$
$$
f_4=\langle S^1S^3\rangle_0,\ f_5=\langle S^1S^6\rangle_0,\ f_6=\langle S^1S^9\rangle_0,
$$
$$
f_7=\langle S^2S^3\rangle_0,\ f_8=\langle S^2S^6\rangle_0,\ f_9=\langle S^2S^8\rangle_0.
$$

The extension of these equations to the case when the magnetic field is nonzero is straightforward and follows the discussion given in Ref. 1. The resulting equations are similar to the above but more complicated and we do not write them down here. We have found by numerical means a fixed-point solution to these equations and the corresponding values of the coordinates (K^*, L^*, M^*) are (0.36946, 0.07978, −0.01875). We find the two relevant eigenvalues are $\lambda_T = 3.007$ and $\lambda_H = 7.927$ as compared to the exact values of $\lambda_T = 3$ and $\lambda_H = 7.845\ldots$. We also obtain the critical temperature to within 2% accuracy, finding $K_c = 0.4302$ as compared to the exact value[7] of $0.4407\ldots$. (See Table I.)

We summarize by making a few observations about the present work. To begin with, our values of λ_T and λ_H lead to $\nu = \ln 3/\ln\lambda_T = 0.998$ and $\delta = (a_H - 1)^{-1} = 16.3$ (where $a_H = 2\ln 3/\ln\lambda_H$) as compared to the exact values of 1 and 15, respectively. The fact that the 1% precision in the determination of λ_H does not lead to a corresponding accuracy in δ follows from the relation $\delta = (a_H - 1)^{-1}$, which implies that $d\delta/\delta = -(\delta+1)da_H/a_H$. Hence a small error in the determination of a_H results in a $(\delta+1)$ times larger error in determining δ. Fortunately the situation is different for α. Secondly, we compare our results for the square lattice which yield 0.2% and 1.1% precision for λ_T and λ_H, respectively, to the best results for the triangular lattice, namely the seven-cluster approximation, for which λ_T and λ_H were obtained to a precision of 1.6% and 0.05% respectively. We see that the second-order cumulant expansion does not suffer very badly by comparison, particularly if one takes into account the much greater simplicity and ease of calculation of a cumulant calculation. Finally, we mention several interesting questions which remain to be answered. Firstly, is the cumulant expansion used here a convergent one, or is it an asymptotic expansion as is the case[5] with the ϵ expansion? Some insight into this question would be gained by a third-order calculation which although considerably more complicated than in second order is presently being carried out. Secondly, as a practical question one would like to know how increasing the cell size affects the accuracy of the calculation. Is there, for example, some optimum cell size for a given order of the cumulant expansion? A systematic investigation of this problem is currently under way.

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