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Study of the cumulant expansion for renormalization transformations on two- and three-dimensional Ising models

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The Niemeijer–Van Leeuwen cumulant expansion is used in the renormalization-group analysis of the critical-point behavior of the Ising model. Second- and third-order results are obtained for the simple cubic and square lattices, respectively, for a variety of cell sizes, using a parameter-dependent renormalization transformation introduced by Kadanoff and Houghton. Although the results in two dimensions are in general good, there is no evidence of any convergence, with the best values for the critical exponents and critical temperature being given by the second-order theory. In three dimensions the values found for the critical temperature and magnetic scaling index for a cell of 27 spins are reasonable, but the corresponding thermal scaling index is quite poor.

I. INTRODUCTION

Considerable progress in the renormalization-group theory of critical phenomena has been achieved using real-space renormalization transformations introduced originally by Niemeijer and Van Leeuwen[1-3] and extended by Kadanoff *et al.*[4,5] All of the calculational methods employed in these real-space analyses involve truncation schemes in which the error involved in the truncation is essentially unknown. This in spite of the extremely impressive accomplishments of these methods, in particular the variational approach of Kadanoff,[4] a fundamental understanding of the nature of these approximations has not yet been obtained.

One of the simplest and perhaps most systematic of these calculational methods is the cumulant expansion originally introduced by Niemeijer and Van Leeuwen[1] in their study of the two-dimensional Ising model on a triangular lattice. Their expansion was essentially in powers of the near-neighbor coupling between spins in different adjacent cells (each with three spins) and gave a qualitatively good description of the ferromagnetic critical point. This method was subsequently applied[6] to the square lattice and gave quite reasonable quantitative results for a cell of nine spins. The cumulant expansion has also been extended to several other problems, including the random-bond Ising model,[7] the self-avoiding walk,[8] the triplet-spin Ising model,[9] and the XY model.[10-12] In general the method gives a reasonable qualitative and in some cases good quantitative solution of these problems.

In view of the simplicity and reasonable success of the cumulant expansion, it seems worthwhile to examine in more detail the nature of this truncation scheme, to examine its possible convergence, if any, and to explore the effects of changing the unperturbed Hamiltonian by changing the cell size. Some work in this direction has already been carried out by Hemmer and workers[13,14] who have calculated the second- and third-order cumulant-expansion results for the magnetic and thermal eigenvalues, respectively, for the triangular Ising model and cells of either three or seven spins. Their overall conclusions are that the cumulant expansion seems to be asymptotic, and that there is possibly an optimal cell size for a given order of the calculation. We have extended this investigation to the square and simple-cubic lattices, respectively, using a parameter-dependent renormalization transformation introduced originally by Kadanoff and Houghton.[15] In Sec. II we present a summary of the formalism and of two possible criteria for determining the "best value" of the parameter. We note that in our approximation scheme this value corresponds to the transformation introduced originally by Neimeijer and Van Leeuwen. In Secs. III and IV we give the results for the two- and three-dimensional Ising model. We make some concluding remarks on the cumulant expansion in Sec. V.

II. BRIEF REVIEW OF THE FORMALISM

In this section we summarize some well-known facts[3] about the renormalization transformation and the cumulant expansion. We consider a set of lattice points with the site spin variable $\sigma_i = \pm 1$ at each site i. The Hamiltonian for the system, $H(\sigma)$, in units of $-k_B T$ can be written

$$H = \sum_i K_i \sum_{\vec{r}} S_i(\vec{r}) , \tag{1}$$

where $\vec{r}$ sums over all lattice sites, $S_i(\vec{r})$ are functions of site spins σ_i in the vicinity of $\vec{r}$, and K_i is the corresponding interaction constant. A renor-

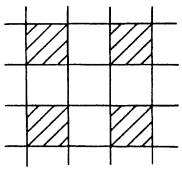

FIG. 1. Schematic representation of sites and cells on a square lattice for a 2×2 cell.

malization transformation can be written

$$e^{H'(\mu)}=\sum_{\sigma} T(\mu,\sigma)e^{H(\sigma)}, \tag{2}$$

which transforms the site spin Hamiltonian $H(\sigma)$ to the cell spin Hamiltonian $H'(\mu)$ on a new lattice whose lattice constant is l times larger than the original lattice, where σ and μ denote the set of old and new Ising spins, respectively. A schematic representation of sites and cells of size 2×2 on a square lattice is shown in Fig. 1. Since H' is in general of the same form as H, but with different interaction constants $K_i'(\{K_j\})$, the renormalization transformation equations can be considered to be

$$K_i'=R_i(\{K_j\}). \tag{3}$$

Linearizing around the fixed point $K_i'=K_i^*$, one has

$$K_i'-K_i^*=\sum_j T_{ij}(K_j-K_j^*), \tag{4}$$

where

$$T_{ij}=\left(\frac{\partial K_i'}{\partial K_j}\right)_{K^*}. \tag{5}$$

The scaling indices and left eigenvectors of T_{ij} are denoted by

$$\sum_i \phi_i^n T_{ij}=l^{y_n}\phi_j^n, \tag{6}$$

where y_T and y_h are the largest thermal and magnetic scaling indices, respectively, and determine the critical indices through such relations as

$$\alpha=2-d/y_T \tag{7}$$

and

$$\delta=y_h/(d-y_h). \tag{8}$$

We will choose $T(\mu,\sigma)$ in the renormalization transformation [Eq. (2)] to be

$$T(\mu,\sigma)=\prod_a \frac{1}{2}\left[1+\mu_a\tanh\left(p\sum_{i\in a}\sigma_i\right)\right] \tag{9}$$

as originally introduced by Kadanoff and Houghton,[15] where $\mu_a=\pm1$ denotes the cell spin variable for cell a and the product is over all cells. In the limit $p\to\infty$, $T(\mu,\sigma)$ reduces to the original Niemeijer–Van Leeuwen transformation

$$T(\mu,\sigma)=\prod_a \frac{1}{2}\left[1+\mu_a\,\mathrm{sgn}\left(\sum_{i\in a}\sigma_i\right)\right]. \tag{10}$$

Generally different values of p define different renormalization transformations. In an exact calculation the scaling indices should be independent[16,17] of p, but in an approximate calculation they will vary with p. Thus the problem arises as to how to choose the "best" p. An extensive discussion of different possible criteria, all valid for an exact calculation, has been given by Bell and Wilson,[17] but we will first consider one proposed by Kadanoff and Houghton.[15] This criterion follows from an analysis of the relation between the site spin and cell spin-correlation functions, i.e.,

$$\langle\mu_a(\vec{r}_a')\,\mu_b(\vec{r}_b')\rangle_{H'}$$

$$=\left\langle\tanh\left(p\sum_{i\in a}\sigma_i\right)\tanh\left(p\sum_{j\in b}\sigma_j\right)\right\rangle_H. \tag{11}$$

Since one can expand any function of the local σ_i in terms of a basis,

$$\tanh\left(p\sum_{i\in a}\sigma_i\right)=\sum_i W_i(p)S_i(\vec{r}_a), \tag{12}$$

it follows from the analysis of Kadanoff and Houghton using the relation between the "eigenoperators" and the S_i that in the exact theory one has

$$l^{d-y_h}=\sum_i \frac{W_i(p)\phi_i^h}{\phi_1^h}. \tag{13}$$

Thus one can use this equation as a second independent method of calculating y_h. This solution will be called Y_h from now on. In the exact theory this must yield the same scaling index as that calculated from linearizing the recursion equations [Eq. (3)], but in an approximate calculation both scaling indices depend on p and in general differ. One could therefore choose as the "best" p its value for which the two scaling indices are the same. If there does not exist such a p, one could alternatively choose the "best" p as the value for which the difference between y_h and Y_h is a minimum. Unfortunately, as we will see in Secs. III and IV, the difference between these two scaling indices as calculated via the cumulant expansion is relatively large in most cases. Whether the lack of an intersection for the two curves $y_h(p)$ and $Y_h(p)$ is an indication that the cumulant expansion determines the eigenvectors $\phi_i^h(p)$ rather poorly is not clear. In lieu of being able to apply the Kadanoff-Houghton criterion we therefore use an alternative one, originally proposed by Bell and Wilson.[17] Their suggestion is based on the possibility of finding a range of p for which the indices essentially remain constant in which case one chooses these values for the indices. In our case

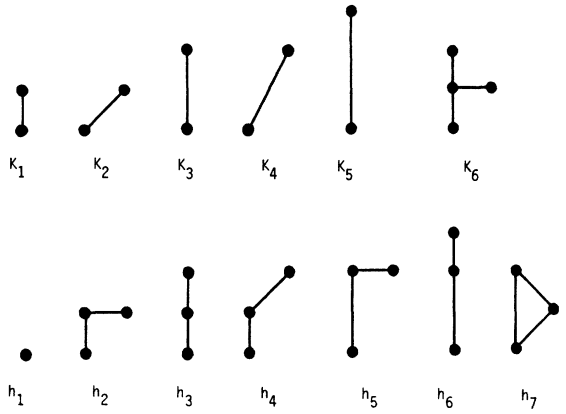

FIG. 2. Diagrammatic representation of interactions up to third-order cumulant expansion for the square lattice.

the p dependence is quite small over a wide range of p extending to infinity and we choose the $p \to \infty$ results as our "best" values.

In the cumulant expansion one writes the Hamiltonian as the sum of two terms

$$H = H_0 + V \,, \tag{14}$$

where H_0 includes only interactions within each cell and V includes only interactions between cells. The latter is then treated as a perturbation. If we denote

$$\langle A \rangle_0 = \Big(\sum_\sigma AT(\mu, \sigma) e^{H_0(\sigma)} \Big) \Big/ Z_0(\mu) \,, \tag{15}$$

where

$$Z_0(\mu) = \sum_\sigma T(\mu, \sigma) e^{H_0(\sigma)} \,, \tag{16}$$

then the basic recursion equations are determined from

$$e^{H'(\mu)} = Z_0(\mu) \langle e^V \rangle_0 \,. \tag{17}$$

The cumulant expansion then yields

$$H' = \ln Z_0 + \langle V \rangle_0 + (1/2!)(\langle V^2 \rangle_0 - \langle V \rangle_0^2) + (1/3!)(\langle V^3 \rangle_0 - 3\langle V^2 \rangle_0 \langle V \rangle_0 + 2\langle V \rangle_0^3) + O(V^4) \,. \tag{18}$$

Further details about the cumulant expansion are given in Refs. 1 and 3.

III. TWO-DIMENSIONAL ISING MODEL ON A SQUARE LATTICE

We have evaluated the recursion equation through third order in the cumulant expansion in Eq. (18) for three different cell sizes, 2×2, 3×3, and 4×4. These nonlinear equations for K_i are complicated and will not be written here.[18] The different types of interactions which arise in this third-order perturbation expansion are represented diagrammatically in Fig. 2, in which the odd and even interactions are explicitly denoted by h_i and K_i, respectively. A typical fixed-point solution for the third-order equations is

$$K^* = (0.3297, 0.1198, -0.0122, -0.0037, 0.0001, 0.00253)$$

for the 2×2 cell in the limit $p \to \infty$.

As we noted earlier our "best" results occur in the limit $p \to \infty$, so we will discuss these first. The results for the scaling indices y_T and y_h as well as the critical temperature as given by K_c are listed in Table I for the three different cell sizes considered. The following results are worth noting. First, the most accurate results are given by the second-order theory, where the scaling indices for both the 3×3 and 4×4 cells agree with the exact results to within 1%. Second, there is no evidence of convergence, since the third-order results are somewhat poorer than the corresponding second-order results. Third, the critical temperature is given accurately for all cell sizes in both second- and third-order perturbation theory and seems to be a relatively insensitive test of the calculation. We should also note that K_c is obtained from Eq. (4). Finally, the best values of the critical exponents determined in this work are given in Table II, where the results of other calculations are also listed for comparison.

We conclude by discussing the effect of the parameter p in the transformation. A characteristic result is displayed in Fig. 3 in which the results for the scaling indices y_T, y_h, and Y_h as determined from Eqs. (6) and (13) are plotted as a function of p. One finds in this case that the difference between y_h and Y_h does not vanish. Although this

TABLE I. Two-dimensional results for y_T, y_h, and K_c for 2×2, 3×3, and 4×4 cells in the limit $p \to \infty$.

Cell size	Order of perturbation	y_T	y_h	K_c
2×2	1	1.006	2.146	0.5186
	2	1.051	1.979	0.4300
	3	1.072	1.975	0.4319
3×3	1	0.927	1.943	0.4697
	2	1.002	1.884	0.4302
	3	1.080	1.899	0.4314
4×4	1	0.932	1.914	0.4607
	2	1.009	1.883	0.4330
	3	1.083	1.914	0.4305
Exact		1.0	1.875	0.4407

TABLE II. Two-dimensional critical indices obtained by present work, Kadanoff and Houghton, and Sudbø and Hemmer (from their second-order results for a cell of seven spins). Scaling laws are assumed in determining these critical indices.

	α	β	γ	δ	η	ν
Present work	0.018	0.116	1.75	16.1	0.234	0.991
Kadanoff and Houghton	0.000 07	0.124	1.75	15.1	0.249	0.999 96
Sudbø and Hemmer	0.134	0.113	1.64	15.5	0.242	0.932
Exact	0	0.125	1.75	15	0.25	1

difference decreases as the order of perturbation increases, it is still very large for a wide range of p. It therefore does not seem sensible to use the Kadanoff-Houghton criterion, as noted earlier.

IV. THREE-DIMENSIONAL ISING MODEL ON A SIMPLE-CUBIC LATTICE

In this section we present the second-order cumulant expansion results for two different cell sizes, $2\times2\times2$ and $3\times3\times3$, respectively. The cumulant expansion for the $3\times3\times3$ cell is not a practical way of performing a renormalization-group calculation since it involves evaluating sums over 2^{27} states, but the program has been carried out as an overall test of the method. The method of solving such problems is outlined in Ref. 18 and no details will be given here. The interactions generated in a second-order calculation are K_2, K_3, h_2, h_3 as are shown in Fig. 2.

In three dimensions the "best" results again correspond to the limit $p\to\infty$. These results for y_T, y_h, and K_c are listed in Table III. The second-order perturbation theory for the $3\times3\times3$ cells yields quite a good K_c and a reasonable y_h as compared with the expected values from series expansions.[19] However, the thermal scaling index is quite poor in all of the calculations and yields a nondiverging specific heat whose first derivative diverges. The corresponding critical exponents for the $3\times3\times3$ cell are listed in Table IV, together with the series-expansion results and the results obtained by the Kadanoff variational meth-

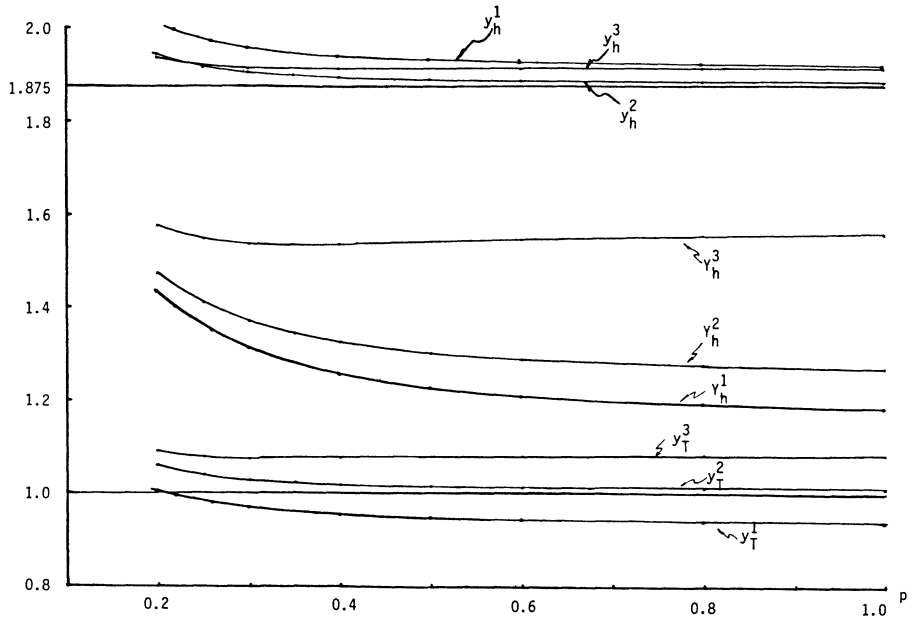

FIG. 3. Scaling indices of 4×4 cells vs p. Superscripts denote the order of cumulant expansion.

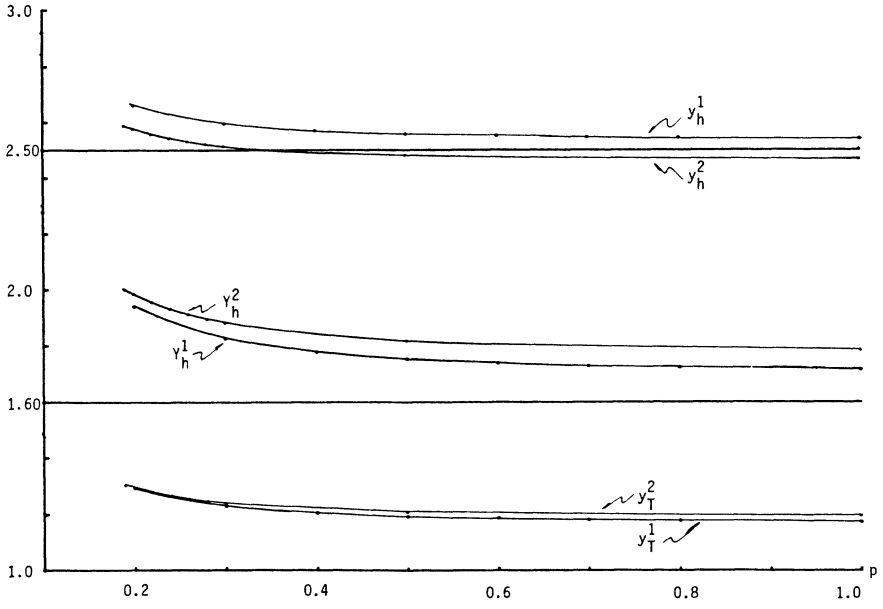

FIG. 4. Scaling indices of $3\times3\times3$ cells vs p. Superscripts denote the order of cumulant expansion.

od. The dependence of the scaling indices on the parameter p is shown for $3\times3\times3$ cells in Fig. 4.

V. COMMENTS

The overall conclusions about this work have already been given in Sec. I and in more detail in Secs. III and IV. It might be worthwhile here, however, to make some general remarks about the cumulant expansion. First, there is no evidence at the moment to suggest that the cumulant expansion in its present form converges. Second, the calculational procedure of treating the higher-order interaction constants self-consistently as suggested originally by Niemeijer and Van Leeuwen seems valid since the fixed-point values of these interactions are correspondingly small with respect to the nearest-neighbor value. Third, the nature of the perturbation expansion imposes a rather severe truncation of the recursion equations for the interaction constants. This limitation is quite possibly the reason for the poor thermal eigenvalue obtained in all of our three-dimensional calculations, since even for the $3\times3\times3$ second-order calculation there are only three interaction constants in zero magnetic field. Finally we would like to comment on a fundamental problem involved in all of these real space calculations, namely, the difficulty involved in estimating the error associated with a particular truncation. In this regard the variational approach seems to be better since one can show[5] that the error in the free energy is of second order in the coupling constants. This is essentially owing to the fact that in this approach one "moves interactions around" rather than simply dropping them. On the other hand, in its present form the error involved in the cumulant truncation scheme is, loosely speaking, first order in the interaction constants since some interactions are simply set equal to zero in a given order of calculation.

TABLE III. Three-dimensional results for y_T, y_h, and K_c for $2\times2\times2$ and $3\times3\times3$ cells in the limit $p\to\infty$.

Cell size	Order of perturbation	y_T	y_h	K_c
$2\times2\times2$	1	1.246	2.788	0.2978
	2	1.209	2.599	0.2468
$3\times3\times3$	1	1.165	2.531	0.2599
	2	1.185	2.455	0.2371
Series expansion results (Ref. 19)		1.60	2.50	0.2217

TABLE IV. Three-dimensional critical indices obtained by present work and variational calculations. Scaling laws are assumed.

	α	β	γ	δ	η	ν
Present work	−0.532	0.460	1.61	4.50	0.09	0.844
Variational	0.113	0.337	1.21	4.60	0.07	0.629
Expected	0.125	0.31	1.25	5.0	0.04	0.64

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