Lattice renormalization group and the thermodynamic limit*

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Recent lattice-renormalization-group calculations have investigated the effect of placing arbitrarily large numbers of spins into blocks, via Monte Carlo numerical methods. These calculations indicate that, in the thermodynamic limit, the fixed point of the recursion relation converges to the exact critical temperature, even though the recursion relations themselves become nonanalytic. It is the purpose of this note to explain why this occurs.

I. INTRODUCTION

A major unsolved problem in lattice-renormalization-group theory is to understand the nature of the truncation involved when only a finite number of spins are used to generate approximate recursion relations. Clearly, the first question in this regard is whether critical temperatues and exponents, say, obtained in a truncated calculation, converge to exact values as more spins are included. No rigorous answer has ever been given to this question, even for the two-dimensional Ising model, although the numerical evidence[1] makes one extremely optimistic. In general, of course, the answer must depend on the specific transformation one has in mind; if there is a nonempty set of "good" transformations, one would like to know rates of convergence so as to be able to give error assignments to predicted exponents.

How does one include more and more spins in a typical (cluster) lattice calculation? In principle, there are two choices: either one introduces more and more blocks of spins, or one places more spins into a given (finite) number of blocks. The first choice is the canonical one for a large variety of good reasons, such as the maintenance of analyticity in the recursion relations and the iterability of these relations necessary for their interpretation. In the second choice, blocks could become arbitrarily large and, hence, critical. This is definitely against the spirit of the whole approach as first conceived by Wilson, Kadanoff, and Niemeijer and van Leeuwen. Nevertheless, it is the second scheme that we consider here for two reasons: (i) Recent Monte Carlo calculations by the author, and by Friedman and Felsteiner,[2] suggest strongly (in two dimensions, anyway) that critical temperatures do, in fact, converge to exact values in the limit of including an infinite number of spins. There is also suggestive, although weaker, evidence for the convergence of exponents. Because the Monte Carlo approach[3] to these calculations is so trivial to perform and labor saving, this peculiar way of obtaining accurate results could well become commonplace and so one is forced to consider it seriously. (ii) There are simple arguments by which one can understand this convergence of critical temperatures, in marked contrast to the canonical schemes. Thus, one hopes that this particular "pathological" type of renormalization may shed some light on the usual schemes and the unanswered questions that we raised earlier.

In Sec. II we present some numerical evidence indicating this convergence of critical temperatures discussed above, and in Sec. III we discuss why things work out the way they do. We conclude with some unanswered questions and speculations in Sec. IV.

II. NUMERICAL EVIDENCE

The class of renormalization-group transformations that we want to consider are defined on an Ising-model partition function. We consider a finite system $\Omega(N)$ consisting of two neighboring hypercubes, each consisting of N^D spins $\sigma_{\vec{i}}=\pm1$, situated on the sites $\vec{i}$ of a simple hypercubic lattice in D dimensions. The two hypercubes are called block 1 (B1) and block 2 (B2). The Ising Hamiltonian is

$$\mathcal{H}_{\Omega(N)}=K\sum_{\vec{i}}\sum_{\vec{\delta}}\sigma_{\vec{i}}\sigma_{\vec{i}+\vec{\delta}}\,, \tag{1}$$

where the sums range over all sites $\vec{i}\in\Omega(N)$ and all nearest-neighbor vectors $\vec{\delta}$, each bond counted once, and periodic boundary conditions are used at the surfaces of $\Omega(N)$.

The transformation from the site spin Hamiltonian of Eq. (1) to a block spin Hamiltonian, defined on two block spins $s_1=\pm1$, $s_2=\pm1$, is made by a transformation kernel $T(s_1,s_2;\{\sigma_{\vec{i}}\})$. We parametrize T by the following functional form:

$$T(s_1,s_2;\{\sigma_{\vec{i}}\})=\tfrac{1}{4}[1+s_1f(m_1)][1+s_2f(m_2)]\,, \tag{2}$$

where f is an odd function of its argument, to be specified, and we restrict ourselves here to arguments that are the magnetization operators for the blocks. That is,

$$m_1 = \frac{1}{N^D} \sum_{\vec{i} \in B1} \sigma_{\vec{i}} \quad \text{and} \quad m_2 = \frac{1}{N^D} \sum_{\vec{i} \in B2} \sigma_{\vec{i}}$$

The partition function sum is then

$$Z_{\Omega(N)} = \sum_{\{\sigma\}} e^{\mathcal{H}_{\Omega(N)}} = \sum_{s_1=\pm 1} \sum_{s_2=\pm 1} \sum_{\{\sigma\}} T(s_1, s_2; \{\sigma\}) e^{\mathcal{H}_{\Omega(N)}} . \tag{3}$$

Now, if one does the sum over $\{\sigma\}$ first in Eq. (3), a function of $s_1 s_2$ must result. This function is generally written in exponential form, so as to suggest a block spin Hamiltonian. That is we have

$$Z_{\Omega(N)} = \sum_{s_1=\pm 1} \sum_{s_2=\pm 1} C_N(K) \exp[q K_N'(K) s_1 s_2] ,$$

where the two functions $C_N(K)$ and $K_N'(K)$ are uniquely defined once we specify q. One wants to interpret $K_N'(K)$ as a new nearest-neighbor coupling for the block spins; q represents the ambiguity in assigning "boundary" conditions to this two-block system. In our numerical work, we take $q = 1$; Friedman and Felsteiner[2] take $q = 2D$. We show, in Sec. III, that the convergence of critical temperatures is unaffected by one's choice of q, as long as it is a positive number. Thus, for the moment, let us leave q as an arbitrary parameter. Then, one obtains the recursion relation from Eqs. (2) and (3)

$$K_N'(K; q) = (1/q) \operatorname{arctanh} \langle f(m_1) f(m_2) \rangle_{\Omega(N)} , \tag{4}$$

where the thermal average is the usual canonical average with respect to $H_{\Omega(N)}$. Shown in Fig. 1 are numerical results obtained for the function $K_N'(K; 1)$, where $D = 2$ and the function $f(x)$ corresponds to the majority rule: $f(x) = \operatorname{sign}(x)$. One sees that for each $N = 3, 5, 7, \ldots$ there is a fixed point K_N^*, defined by $K_N'(K_N^*) = K_N^*$. Heuristic arguments (see below) suggest that one should plot K_N^* vs N^{-1} and this is shown in the same figure. These results were obtained by the standard Metropolis Monte Carlo method to evaluate the thermal average on the right-hand side of Eq. (4); thus, there is a statistical error in all of the plotted points shown that is, we estimate, roughly twice the size of the data points. A straight line drawn through the fixed point values is seen to intersect the K^* axis near the exact Ising critical temperature $K_c = 0.44068\ldots$. Moreover, one can define a thermal eigenvalue $\nu(N)$ via $dK_N'/dK|_{K_N^*} = N^{1/\nu(N)}$, and very slow convergence toward $\nu(\infty) = 1$ is suggested by the data (not shown). Friedman and Felsteiner[2] report similar findings with the following notable difference: their choice of $q = 2D$ produces much more rapid convergence toward K_c and they report values of K_N^* accurate to four figures, in contrast to the roughly two-figure accuracy here. [They suggest $(\ln N)^{-1}$ convergence of $\nu(N)$.] No extensive data are available for $D = 3$.

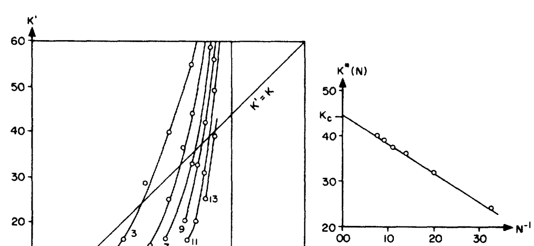

FIG. 1. Recursion relation $K_N'(K;1)$ for various odd N, and fixed point values K_N^* plotted vs N^{-1}. These results are for the two-dimensional Ising model, but similar plots for K_N' are obtained in any dimension $D \geq 2$.

From the figure, one sees that the recursion relations, Eq. (4), may be tending toward, as $N \to \infty$,

$$K_\infty'(K; q) = \begin{cases} 0 & K < K_c , \\ \infty & K > K_c , \end{cases} \tag{5}$$

where K_c is the exact critical value. This is a loss of analyticity indeed!

III. UNDERSTANDING THESE RESULTS

In this section we want to present heuristic arguments for the above specific results for the majority rule transformation, and what one might expect for more general transformations. First, one expects $K_\infty'(K) = 0$ for $K < K_c$ for a wide class of transformations because the correlation length is being rescaled by N under a single iteration of Eq. (4) when N is finite: $\xi' = \xi/N$. Thus, if $K < K_c$, then ξ is finite and so $\xi' \to 0$ as $N \to \infty$. So, the new block system is characteristic of zero correlation length and this means $K' = 0$. For $K > K_c$, things are more subtle. For the majority rule, anyway, one is seeing a single iteration map the system to its completely ordered zero-temperature state and this is $K' = \infty$. So, one way to think about the above results is that a single iteration of the recursion relations, for very large N, roughly reproduce the result of a large number of iterations of the recursion relations for small N, albeit with a shifting of the fixed point value toward K_c.

The rate of convergence of these fixed point values K_N^* toward K_c is consistent with what one might expect from the usual[4] argument that nothing special happens until the correlation length reaches the edge of the system. More specifically, one makes a finite-size scaling ansatz for the correlation length, appropriate when $N \gg 1$ and $|K - K_c| \ll 1$, via

$$\xi_N(K) \sim N\Phi(|K - K_c| N^{1/\nu}),$$

where the function $\Phi(x)$ may depend on the sign of $K - K_c$, and should be analytic near $x = 0$ and fall off like $x^{-\nu}$ at large x. Then, postulating that the fixed point $K_N^*(q)$ occurs only when the correlation length is some nonzero percentage of N, say $c(q)N$, where $c(q) > 0$, one solves

$$c(q) = \Phi(|K_N^*(q) - K_c| N^{1/\nu}).$$

If there exists a positive $x_0(q)$ of order unity such that $\Phi(x_0) = c$, then we have, as $N \to \infty$,

$$K_N^*(q) \approx K_c \pm x_0(q) N^{-1/\nu}, \tag{6}$$

where the sign distinguishes convergence from below or above. Since $\nu = 1$ for $D = 2$, Eq. (6) is a possible explanation for my data. [For Friedman and Felsteiner's data, apparently $x_0(2D) = 0$, and a larger power of N^{-1}, ignoring possible $\ln N$ behavior, governs convergence.] If more results were available in three dimensions, where $\nu < 1$, then Eq. (6) could be tested more critically.

The numerical results have been for the majority rule $f(x) = \mathrm{sign}(x)$. However, let us now generalize to any odd function $f(x)$ that is, at most, discontinuous in a finite number of places. We would like to conjecture that in the thermodynamic limit, $N \to \infty$, Eq. (4) becomes for $K \neq K_c$

$$K'_\infty(K; q) = (1/q)\,\mathrm{arctanh}\{[f(m_s(K))]^2\}, \tag{7}$$

where $m_s(K)$ is the spontaneous magnetization, and one defines $f(0) = 0$ for those odd functions, such as the majority rule, that are discontinuous at the origin. [If f is discontinuous elsewhere, take the Eq. (7) to be true everywhere except where $m_s(K)$ equals these discontinuity points.] If Eq. (7) is correct, it has a number of interesting consequences. First, one sees that no analytic function produces the convergence of fixed points; i.e.,

$$\lim_{N\to\infty} K_N^*(q) \neq K_c .$$

To see this, take the linear transformation, for example, $f(x) = x$. If there is a nonzero fixed point of Eq. (7), it will be strictly greater than K_c. Any other analytic function behaves in the same way. In fact, if we require $f(x)$ to be nondecreasing in the interval $-1 \le x \le 1$, then the "correct" behavior of Eq. (5) can only be realized by $f(x) = \mathrm{sign}(x)$. Also, one sees for this particular function why one obtains Eq. (5) for any positive q.

We do not have a rigorous proof of Eq. (7), but we do have the following heuristic argument. First, we restrict ourselves to analytic odd $f(x)$, which may be used to approximate piecewise discontinuous functions arbitrarily closely (in the sense of some idea of closeness that we do not specify.) Then, we automatically have $f(0) = 0$, and we may also expand $f(x)$ in an odd power series, and we argue for a sort of "factorization" of correlations term by term; that is, we would like to be able to show

$$\lim_{N\to\infty} \langle m_1^r m_2^s \rangle_{\Omega(N)} = [m_s(K)]^{r+s}$$

for odd integers r and s. For example, take $r = s = 1$. Then, because we have a sum of correlation functions with an even number of spins (two), the function $\langle m_1 m_2 \rangle$ is even in h if we add a magnetic field term

$$h \sum_{\vec{i} \in \Omega(N)} \sigma_{\vec{i}}$$

to the Hamiltonian. Because it is even in h, it is plausible that this correlation function will be continuous as $h \to 0$, *after* $N \to \infty$, even if $K > K_c$. Assuming this is correct, we may evaluate the original function via this particular limit; i.e.,

$$\lim_{N\to\infty} \langle m_1 m_2 \rangle_{\Omega(N)} = \lim_{h\to 0} \lim_{N\to\infty} \left(N^{-2D} \sum_{\vec{i} \in B1} \sum_{\vec{j} \in B2} \langle \sigma_{\vec{i}} \rangle \langle \sigma_{\vec{j}} \rangle + N^{-2D} \sum_{\vec{i} \in B1} \sum_{\vec{j} \in B2} (\langle \sigma_{\vec{i}} \sigma_{\vec{j}} \rangle - \langle \sigma_{\vec{i}} \rangle \langle \sigma_{\vec{j}} \rangle) \right), \tag{8}$$

where the thermal averages on the right-hand side of Eq. (8) are now with respect to the Hamiltonian augmented with the above magnetic field term. Now the second double sum in Eq. (8) can be expected to go to zero like $A(K)N^{-D}$, where $A(K)$ is finite for $K \neq K_c$, because of the exponential decay of the correlation function $\langle \sigma_{\vec{i}} \sigma_{\vec{j}} \rangle - \langle \sigma_{\vec{i}} \rangle \langle \sigma_{\vec{j}} \rangle$ at large separations $|\vec{i} - \vec{j}|, K \neq K_c$. This leaves

$$\lim_{N\to\infty} \langle m_1 m_2 \rangle_{\Omega(N)} = [m_s(K)]^2$$

from the first term alone, again with $K \neq K_c$. For higher powers of r and s one can add and subtract terms to produce the connected n-point correlation functions. Then, under identical assumptions about (i) continuity at $h = 0$ for even correlations, and (ii) exponential decay of the connected correlations, one achieves the above "factorization," which would establish Eq. (7) [for analytic $f(x)$, anyway].

IV. CONCLUSIONS

We have presented heuristic arguments which explain the convergence of critical temperatures in certain renormalization group transformations in the thermodynamic limit, under plausible assumptions. One interesting result was that for a fairly wide class of transformations, given by Eq. (2), only the majority rule produced convergence to the exact critical temperature, if Eq. (7) is correct. One wonders if the canonical schemes can be as restrictive in the admission of "good" transformations. One might also speculate that Eq. (6), for the rate of approach of critical temperatures, could also have wider applicability where N would be interpreted (in the usual schemes) as the width of the entire (finite) cluster. This is possible because, even in the canonical methods, there are always (small) couplings which sample the collective behavior of the entire system. Finally, it is clear that the above arguments for Eq. (7) could equally well be applied to the slighly more general situation of an arbitrary finite number of blocks, as the size of the smallest block tends to infinity in a thermodynamic way. This would then suggest the convergence of critical lines (hypersurfaces) to exact values in systems with additional coupling constants. An open question is the nature of the convergence of critical exponents in these schemes, and, of course, a more rigorous treatment of the issues we have considered here.

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