

## Tricritical behavior in two dimensions. I. Model-dependent behavior from finite size effects

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The onset of two-dimensional tricritical behavior in  $N \times \infty$  strips of spins in an Ising-like model is investigated. This is done through numerical computation of the largest eigenvalue of the single-spin advance transfer matrix. Primary attention is paid to the specific heat at constant nonordering field. The usual phase diagram, in zero ordering field, locates the tricritical point at the intersection of a first-order line and a  $\lambda$  line; it is found here that a curve of large-field, rounded and bounded specific-heat peaks also seems to intersect this point. This curve, when it exists, may be helpful in experimentally locating tricritical points in any dimension. Evidence is also presented, at zero nonordering field, for the validity of the Onsager specific-heat temperature shift  $N^{-2} \ln N$  in the model.

### I. INTRODUCTION

This is the first of a two-part study of tricritical behavior in two dimensions; here we are concerned with the phase diagram of a particular simple model thought to have a tricritical point. In Paper II, we are concerned with the universal behavior, which we approach via the  $\epsilon = 3 - d$  expansion.

A large variety of real two-dimensional or pseudo-two-dimensional critical systems are known; it is an interesting experimental question as to whether one may find a two-dimensional tricritical system.<sup>1</sup> As far as the author is aware, however, no such systems have been discovered to date.

Theoretically, two-dimensional tricritical systems are interesting because they represent one of the simplest examples of multicritical behavior that is (i) qualitatively different from ordinary critical behavior, and (ii) fluctuation dominated<sup>2</sup> so that non-mean-field behavior is expected. Thus, a better understanding of how mean-field theory is incorrect in two-dimensional tricritical systems can only add to our understanding of the corresponding situation in critical systems in three and two dimensions. A number of questions in this regard come to mind. For example, one of the basic measures of deviations from the classical Ornstein-Zernike theory of correlations is the exponent  $\eta$ , which measures the anomalous behavior of the relevant operator associated with the order parameter. In Ising-like critical systems  $\eta$  is thought to be quite small in three dimensions ( $\sim \frac{1}{20}$ ), but known to be exactly  $\frac{1}{4}$  in two dimensions. Thus, by this measure, we may say that three dimensions is quite "close" to the upper borderline dimension of four (where  $\eta$  is thought to be zero), whereas two dimensions is much farther away.

What should we expect of the tricritical  $\eta$  in two dimensions; i.e., is two dimensions close or far from the upper borderline dimension<sup>2</sup> of three? Other, more general questions involve the validity of phenomenological scaling theories<sup>3</sup> in two dimensions; multicritical scaling functions, in general, and tricritical scaling functions, in particular, must have a very rich structure<sup>4</sup> in order to describe the variety present in the scaling regime. How much of this structure is accessible to the  $\epsilon = 3 - d$  expansion?

There are also some interesting puzzles with regard to the model-dependent properties of specific Hamiltonians. For example, tricritical mean-field theory<sup>5</sup> yields definite predictions about the qualitative variation of the phase diagram with parameters in the Hamiltonian. By "qualitative" we mean things like the existence or absence of a tricritical point. These predictions are in contradiction, sometimes, with one's intuitive notions and approximate lattice renormalization-group calculations.<sup>6</sup> Thus, even the crude behavior of the phase diagram in some simple models is in doubt.

A number of authors have investigated tricritical systems in three dimensions or higher; let us mention those who have done computations that specifically relate to two dimensions. Stephen and McCauley, and Chang, Tuthill, and Stanley have calculated the tricritical exponents  $\eta_t$ ,  $\gamma_t$ , and  $\phi_t$  through leading nontrivial order<sup>7</sup> in  $\epsilon$ . Nienhuis and Nauenberg, and Berker and Wortis have considered two-dimensional tricritical systems with approximate lattice renormalization-group calculations.<sup>6</sup> These two sets of calculations raise the question: is the value of the tricritical crossover exponent  $\phi$ , in two dimensions, larger or smaller than the mean-field value of  $\frac{1}{2}$ ? The lowest-order  $\epsilon$  expansion heads in

one direction (larger) and the finite lattice calculations tend toward the other direction.

We do not claim to resolve all of these matters here, but we do touch on some of them. Let us briefly summarize the results of our investigation here, and in Paper II. Here, we consider a specific Ising-like system. Unfortunately, there is no exactly solvable tricritical analog of the two-dimensional Ising model. Thus, even the existence of a tricritical point in this model and other simple models is not rigorously known, and the evidence for such a point is necessarily indirect. So, we try to discover how a standard tricritical phase diagram<sup>3</sup> may arise out of the thermodynamics of  $N \times \infty$  strips of spins, which we can calculate "exactly" (to eight figures, anyway). As long as  $N$  is finite, no true tricritical behavior can exist; yet there must be a precursor in large specific heats, for example, and that is what we look for. We find that, indeed, the expected precursor to the  $\lambda$  line is well resolved at small  $N$ , but there is less evidence for the first-order line in these specific heats. One thing that we find is that once one adds a coupling to the Hamiltonian that can induce tricritical behavior, the precursor to the  $\lambda$  line ceases to extend down to zero temperature. This is certainly evidence suggestive of a first-order line. On the other hand, we might have expected a clear precursor to  $\delta$  function specific heats on the first-order line; this we do not see. The reason for this may be that the first-order line is very nearly parallel to the temperature axis in the model.

Also, we find that a curve of specific-heat peaks, as a result of paramagnetic disordering at large nonordering field, tends to intersect the  $\lambda$  line in the tricritical region. This curve, of course, is *not* a precursor to a phase boundary, but if it is drawn on the usual phase diagram, we conjecture that it also intersects the tricritical point. This would produce a diagram looking rather like the spin flop or bicritical system.<sup>8</sup> This additional curve might be useful experimentally in more accurately locating tricritical points via calorimetry measurements in any dimension, since one could now identify this point as the intersection of three special lines in zero-ordering field, as opposed to the usual two.

Moreover, we consider quantitatively how the precursor to the  $\lambda$  line approaches the true  $\lambda$  line as  $N \rightarrow \infty$ . A natural guess, away from the tricritical point, is the Onsager result,<sup>9</sup>  $N^{-2} \ln N$ , and we find good evidence for this at zero nonordering field by comparing with high-temperature-series estimates. In general, finite size scaling theory<sup>10</sup> predicts that this temperature shift should be  $AN^{-1/\nu}$ , where the amplitude  $A$  is known to vanish in a variety of situations for the Ising model, leaving the  $N^{-2} \ln N$  correction. Our result here suggests that this resulting leading correction is, in fact, universal. It would be interesting to know what, if any, exponent is associated with

this correction.

In the following paper,<sup>11</sup> we consider the effect of the second nontrivial order in  $\epsilon$  on the calculations of tricritical exponents and we calculate a spin-spin correlation function also. Our series, evaluated at  $d=2$ , yield the estimate  $\eta_t=0.027$  in the Ising case; this is still quite small, but it does represent an order of magnitude increase from the lowest-order term alone. Thus, one wonders if the exact result could be an order of magnitude larger still or should we believe this estimate? In any event, one is led to the conclusion that the lowest order term alone is misleadingly small. The question raised earlier about  $\phi_t$  is answered in a sense; the series is very ill behaved, producing a *negative* estimate at this new order. Presumably, this is incorrect because it leads formally to the conclusion that no crossover occurs; however, one possible interpretation of this result is that the series has "overcorrected" and that the exact  $\phi_t$  is indeed less than  $\frac{1}{2}$  and positive. We also find that, beginning at his new order in  $\epsilon$ , the spherical model limit fails to exist, in sharp contrast to the situation at critical points where not only does this limit exist, but the expansion is convergent in the limit. This is a not unreasonable result, considering the work of Emery,<sup>12</sup> who demonstrated that no tricritical point exists in this limit (in a closely related model) for any  $d < 3$ . These results, and various others, are discussed in detail in the following paper.

In Sec. II of this work we introduce our model and discuss the general approach that we take. In Sec. III we discuss some details of our numerical methods; the reader interested only in our results will find these in Sec. IV. We conclude with a very brief summary in Sec. V.

## II. MODEL

One of the simplest models thought<sup>5,6</sup> to exhibit a standard tricritical phase diagram<sup>3</sup> is defined by the Ising type Hamiltonian ( $\sigma_i = \pm 1$ )

$$H = J \sum_i \sum_{\delta_{nn}} \sigma_i \sigma_{i+\delta} - K \sum_i \sum_{\delta_{nnn}} \sigma_i \sigma_{i+\delta} - h \sum_i \sigma_i, \quad (1)$$

where the sums range over the sites  $i$  of an  $N \times \infty$  square lattice with nearest-neighbor vectors  $\delta_{nn}$  and next-nearest-neighbor vectors  $\delta_{nnn}$ . The boundary conditions we use are discussed below. We are interested in the sector of positive  $J$ ,  $K$ , and  $h$  and the limit  $N \rightarrow \infty$ . This sector generates antiferromagnetic ordering at small fields  $h$  and low temperatures; thus we will refer to  $h$  as either the magnetic field or the nonordering field. By considering what spin configurations minimize  $H$ , where we count each bond once, one sees that the ground state ( $T=0$ ) energy per spin is given by  $-2J - 2K$  for  $h \leq 4J$ , and  $2J - 2K - h$  for  $h \geq 4J$ . There is an abrupt step in

the ground-state magnetization and sublattice (sites generated by  $i + \delta_{nm}$ ) magnetization, as a function of  $h$ , at  $h = 4J$ , the energy is continuous (as a function of  $h$ ) at this point.

Unfortunately, no exact solution exists for the partition function of the Hamiltonian of Eq. (1), or, for that matter, any other similar short-range Ising-like system (in the interesting limit  $N \rightarrow \infty$ ) so as to exhibit the presumed tricritical behavior directly. However, for finite  $N$  we can calculate the free energy from the largest eigenvalue of a finite size matrix, the transfer matrix  $V_N$ . This we do numerically; densities, such as the energy and the magnetization per spin, and response functions, such as the specific heat, may be obtained by differentiation.

When constructing a transfer matrix, one has the two natural choices (among others) of adding either an entire row of  $N$  spins each "time," or adding a single spin. In the simple nearest-neighbor Ising case (when  $K = h = 0$  in our Hamiltonian) these two choices correspond to the different approaches of Onsager<sup>9</sup> and Kramers and Wannier<sup>13</sup> to the same problem. In that case, as is well known, the first choice proved much more analytically tractable. Here, we add a single spin because our numerical approach is more in the spirit of the work of Kramers and Wannier; we want to obtain an extremely sparse matrix. The boundary conditions, then, appropriate for this approach, are that when one reaches the last ( $N$ th) spin in a row, the next neighbor along that same row is taken to be the first spin in the next row. See Fig. 1 for an illustration of how the spins are built up.

Inspection of the partition function sum reveals that for the Hamiltonian of Eq. (1), the single spin advance transfer matrix requires a basis of  $2^{N+1}$  states. This basis is taken to be all the possible assignments of  $\pm 1$  to any "consecutive"  $N + 1$  spins, thinking of the spins as uniformly spaced on the threads of a screw (a helix),  $N$  spins per pitch. Let us denote by  $C$  one such assignment of  $\pm 1$ ; i.e.,  $C = \{\sigma_1, \sigma_2, \dots, \sigma_N, \sigma_{N+1}\}$ , for particular values of the  $\sigma_i$  (see Fig. 1). Each configuration  $C$  may be thought of as an old configuration, which is acted

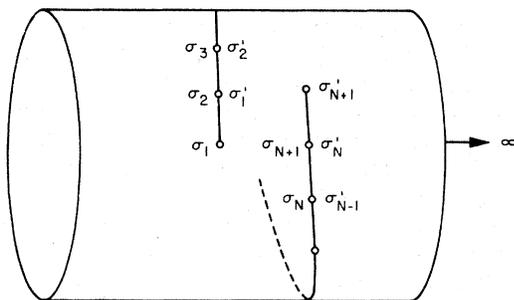


FIG. 1. Labeling of old and new configurations  $C$  and  $C'$  is shown. The spin being added introduces four new bonds.

upon by the transfer matrix via matrix multiplication to generate all possible new configurations  $C' = \{\sigma'_1, \sigma'_2, \dots, \sigma'_N, \sigma'_{N+1}\}$  with certain (relative) probabilities which we specify below. Each new configuration is related to two old configurations and vice versa. The relation is obtained by rotating the old configuration forward along the screw by one spin ( $2\pi/N$ ), dropping one spin from the list, and replacing it by a new spin that may be up or down.

It is convenient to explicitly define this operation of rotation and replacement by introducing two operators  $R_{\pm}$  defined by

$$R_{\pm} \{\sigma_1, \sigma_2, \dots, \sigma_N, \sigma_{N+1}\} = \{\pm 1, \sigma_1, \sigma_2, \dots, \sigma_{N-1}, \sigma_N\} \quad (2)$$

Then, in terms of these operators, the transfer matrix has matrix elements which may be read off from Fig. 1 as

$$V_N(C', C) = x^{\sigma'_{N+1}(\sigma_{N+1} + \sigma_2)} y^{\sigma'_{N+1}(\sigma_1 + \sigma_3)} z^{\sigma'_{N+1}} \times (\delta_{R_+ C', C} + \delta_{R_- C', C}) \quad (3)$$

where  $x = e^{-\beta J}$ ,  $y = e^{\beta K}$ ,  $z = e^{\beta h}$ , and  $\delta_{C', C}$  is a Kronecker  $\delta$  for two configurations  $C'$  and  $C$ . That is,

$$\delta_{C', C} = \delta_{\sigma'_1, \sigma_1} \delta_{\sigma'_2, \sigma_2} \dots \delta_{\sigma'_{N+1}, \sigma_{N+1}}$$

Thus, one sees from Eq. (3) that  $V_N$  has only two nonzero entries for each row and column. As one sees from the construction, this is solely a result of having Ising spins (two spin states) and adding one at a time. It would occur for an arbitrary Ising Hamiltonian in any number of dimensions. On the other hand, the enlarged basis ( $2^{N+1}$  vs  $2^N$ ) is a result of including the next-nearest-neighbor interaction and insisting on adding one spin at a time. The systematic repetitive structure of  $V_N$ , for a particular ordering of the basis states, is shown in Fig. 2. The pseudodiagonal nature of these matrices is deceptively simple, and it is interesting to compare  $V_N$  with the transfer matrix of Ref. 11.

As usual, the free energy per spin  $f$  is determined in the  $N \times \infty$  system by  $-\beta f = \ln \lambda_0$ , where  $\lambda_0$  is the largest eigenvalue of  $V_N$ . Throughout, we will suppress the dependence of  $\lambda_0$  on its parameters  $N$ ,  $x$ ,  $y$ , and  $z$ .

It is very convenient to compute not only  $\lambda_0$  but its associated left and right eigenvectors, which we denote by  $\psi_L$  and  $\psi_R$ . This is because densities may be obtained from the inner product  $\lambda_0' = (\psi_L, V_N' \psi_R)$ , where the prime denotes differentiation with respect to a parameter. As an example, the magnetization per spin  $m$  is obtained by dividing the eigenvectors into upper (+) and lower (-) components, each a vector of  $2^N$  components; that is, one writes  $\psi_R = (\psi_R^+, \psi_R^-)$  and similarly for  $\psi_L$ . Then one finds

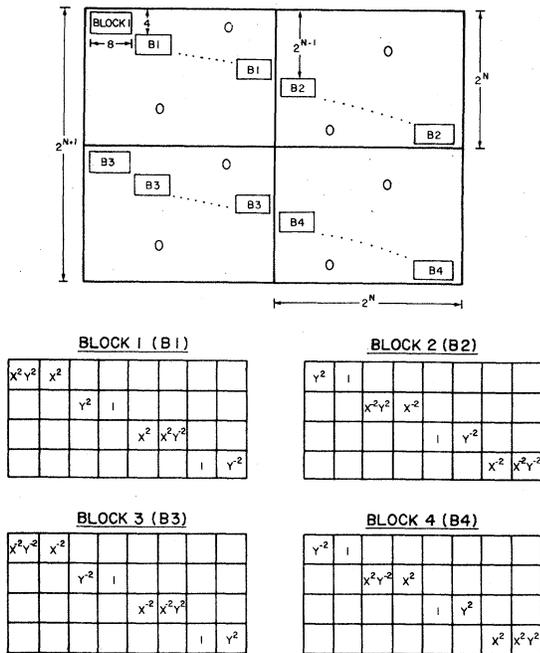


FIG. 2. Repetitive block structure of  $V_N$  for a particular ordering of the basis; every element of block 1 and 2 should be multiplied by  $z$ ; multiply blocks 3 and 4 by  $z^{-1}$ . The ordering is as follows: the first configuration is all spins up; denote this by  $(0, 0, \dots, 0)$ . Then generate all remaining configurations by counting in binary from the left. The next few configurations are  $(1, 0, 0, \dots, 0)$ ,  $(0, 1, 0, \dots, 0)$ ,  $(1, 1, 0, \dots, 0)$ , etc. Down spins are a 1. Blank entries in the blocks are zeros.

that  $m = (\psi_L^+, \psi_R^+) - (\psi_L^-, \psi_R^-)$ . Because  $V_N'$  may always be obtained analytically, densities are obtained to the same numerical accuracy (or greater) as the eigenvalue and vectors. However, response functions require a numerical differentiation.

### III. NUMERICAL METHODS

We obtain the eigenvalue and vectors in the following standard way. We start with an arbitrary right vector and successively multiply by  $V_N$ , rescaling each time, until the vector has become the right eigenvector to a given accuracy (as indicated by its lack of change under multiplication). One final multiplication yields  $\lambda_0$ . Next, we repeat the process for an arbitrary left vector, obtaining the left eigenvector and  $\lambda_0$  again. This provides a consistency check on the eigenvalue.

This can be done for larger and larger widths  $N$  until one runs out of computer storage or time. The ultimate computer storage requirements are, basically, twice the length of a vector with  $2^{N+1}$  entries. (The matrix  $V_N$  is, of course, never stored because it is practically all zeroes; only the multiplication rule is stored.) The basic limitations in computing time with

this method depend on  $N$  in two distinct ways. First, there is just the usual increase because larger systems (column and row vectors) require more elementary multiplications per *single* iteration of the transfer matrix. This effect is completely independent of the underlying thermodynamics. Secondly, one must consider the number of iterations (multiplications by  $V_N$ ) needed to obtain the eigenvalue and vectors to a given, fixed, accuracy. This number is quite sensitive to the values of the parameters because an arbitrary vector turns into the leading eigenvector with an error of  $\text{const} \times (\lambda_1/\lambda_0)^j$  after  $j$  multiplications, where the constant is independent of  $j$ , and  $\lambda_1$  is the second largest eigenvalue (assuming it is real). From Onsager's work,<sup>9</sup> one expects at least two-fold degeneracy of the largest eigenvalue in the ordered phase (in the limit  $N \rightarrow \infty$ ), and infinite degeneracy along the  $\lambda$  line. Thus, one may anticipate, for a fixed finite  $N$  where there is no degeneracy, slower convergence at low temperatures as compared with high temperatures. Also, for the same reason, one expects worse convergence as  $N$  increases at a fixed low temperature. This troublesome effect may be lessened significantly by a standard trick known as Aitken's  $\delta^2$  process,<sup>14,15</sup> which we describe now. Suppose, for a moment, that after  $j$  iterations the *only* error is the leading error  $(\lambda_1/\lambda_0)^j$ . Then, we have precisely geometric convergence; but a geometric series can be summed by a knowledge of only three successive terms. This summation of three successive terms is the  $\delta^2$  extrapolation; it is carried out on the components of the vectors at convenient intervals in the multiplication procedure. The extrapolation has the effect of removing one's best guess for the leading correction. Further corrections, due to other eigenvalues, are responsible, then, for the ultimate convergence rate. Decreases in computing time by factors as large as 6 have been observed with this technique applied here.

Finally, for this section, we mention certain alternate numerical approaches. The simple multiplication is rather crude in the sense that it develops the partition function by, essentially, adding up all the terms until the free-energy density settles down to a desired accuracy. One may argue that it might be better to exploit other special properties of the largest eigenvalue. Specifically, there are a variety of variational techniques for very large symmetric (sparse) matrices.<sup>15</sup> One simple generalization of one of these techniques to the nonsymmetric matrix  $V_N$  is the following. Begin with arbitrary positive trial vectors  $\psi_L^i$  and  $\psi_R^k$ . Then "relax" these vectors one component at a time in order to make  $\lambda^i = (\psi_L^i, V_N \psi_R^k) / (\psi_L^i, \psi_R^k)$  stationary. That is, let the  $q$ th component of  $\psi_L^i$  become  $a_q + \alpha$ , and the  $q$ th component of  $\psi_R^k$  become  $b_q + \beta$ . Then, one has a new estimate  $\lambda_{\text{new}}^i$ . Requiring  $\partial_\alpha(\lambda_{\text{new}}^i) = \partial_\beta(\lambda_{\text{new}}^i) = 0$  results in a determination of  $\alpha$  and  $\beta$  from quadratic equations.

This scheme has been found to converge, but on relatively small matrices (say,  $128 \times 128$  or less) the simple multiplication was faster. However, due to a change in computer, the relaxation scheme was never pursued to very large matrices (say,  $4096 \times 4096$  or larger), and so the optimum method is not known. For completeness, we should mention that for very small matrices (small enough to be stored), both of the above methods are inferior to generating  $V_N^{2j}$  directly by  $j$  matrix multiplications and taking the trace for large enough  $j$ .

For all such methods, one may obtain successive lesser eigenvalues (some may be complex) and vectors, if desired, by appropriate orthogonalization. Thus, investigations of the spectrum and hence, correlation functions, are possible in principle.

#### IV. RESULTS

Essential for the generation of tricritical behavior is the next-nearest-neighbor coupling  $K$  in the Hamiltonian of Eq. (1). Thus, it is instructive to first consider the case when this coupling is absent. As mentioned, we shall deal with the behavior of  $C_h$ , the specific heat.

Shown in Fig. 3 are points in the  $h/J$ - $T/J$  plane where  $C_h$  peaks along lines of constant  $h/J$ . In the computation  $K=0$ ,  $J$  is fixed and positive, and  $N=3$ . As one sees from Fig. 2,  $N=3$  represents the smallest possible realization of the transfer matrix ( $N=2$  is possible in zero field). In Fig. 3, the curve that extends to zero magnetic field is the precursor to the phase boundary ( $\lambda$  line) for a simple antiferromagnet in a magnetic field. From the figure one sees certain "smooth" behavior<sup>16</sup> that one can expect to persist as  $N \rightarrow \infty$ . In particular, one expects a quadratic approach to the  $h=0$  axis, which is certainly a reasonable guess from the figure also. One also sees the precursor to the phase boundary approaching the  $T=0$  axis in an approximately linear fashion, so that smoothness is lost at this point. Also intersecting the  $T=0$  axis at  $h/J=4.0$  is an asymptotically linear curve characterizing disordering in the paramagnetic phase at fields  $h/J \geq 4.0$ . These paramagnetic specific-heat peaks represent the same process that causes specific-heat peaks in the one-dimensional Ising model. Hence, this curve is not a precursor to a phase boundary and one expects  $C_h$  to remain bounded and rounded on this curve as  $N \rightarrow \infty$ . Finally, one sees other maxima in  $C_h$  out at relatively large temperatures and intermediate fields for which we have no particular interpretation. As  $N$  increases one expects, and finds, little change in this basic picture: the precursor to the phase boundary shifts to slightly higher temperatures and the magnitude of the specific heat on this line grows slowly [say  $A(h) \ln M$ ] with  $N$ . Because one can generate exactly solvable models of simple two-dimensional antiferromagnets in a field,<sup>17</sup> there is little point in pursuing

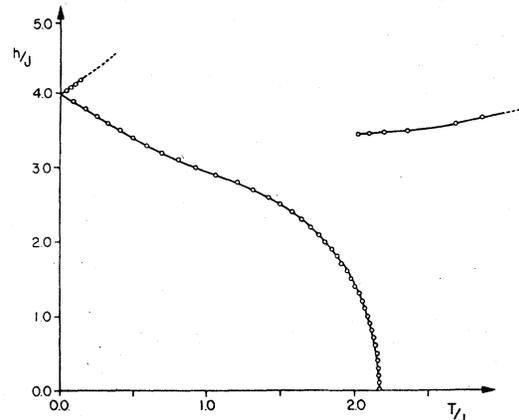


FIG. 3. Points in the  $h/J$ - $T/J$  plane where the specific heat  $C_h$  peaks along lines of constant  $h/J$ . For these results the width  $N=3$  and the next-nearest-neighbor coupling  $K=0$ .

this case via the approach here.

Next, consider the same size system,  $N=3$ , but with the addition of a nonzero next-nearest-neighbor coupling  $K=J/2$ . This is shown in Fig. 4. Now one sees that the large magnetic field and  $\lambda$ -line curves are still intersecting around  $h/J \approx 4.0$  but at a nonzero temperature and with a complicated behavior in this region, which we identify as the tricritical region. This complicated transient behavior, an artifact of small  $N$ , is shown with an increased scale in Fig. 5 for  $N=3, 5$ , and  $7$ . Only odd  $N$  is considered in order to avoid any effects due to antiferromagnetic "mismatch" in the ground state. One sees simple smooth curves arising as  $N$  increases, although it is not at all obvious just exactly what is developing. The points are plotted for equal intervals of  $h/J$ ; thus any apparent "gap" should be interpreted as rapid, but analytic behavior that one would see with an infinitely fine mesh of points.

Let us assume, for the moment, that a tricritical point emerges in the region shown as  $N \rightarrow \infty$ . One of the things that we do not understand is the role played by the first-order line in the specific-heat data for finite  $N$ . Presumably, the energy density undergoes a jump discontinuity across the first-order line in the limit. The amplitude of the jump must vanish as  $T \rightarrow 0$ , if the energy is to be continuous at  $h/J=4.0$ . This implies, by the usual Clausius-Clapeyron equation argument that the first-order line is horizontal at this point if it is differentiable there. However, there is no reason to expect the first-order line to continue to be horizontal for  $T/J$  greater than zero and thus one must anticipate  $\delta$ -function singularities in  $C_h$ ; nevertheless we see little evidence (however, see below) for this at finite  $N$ . This may just be due to the first-order line being very nearly horizontal except when very close to the tricritical point.

In any event, we would like to conjecture the following about those curves that we do see in Figs. 4

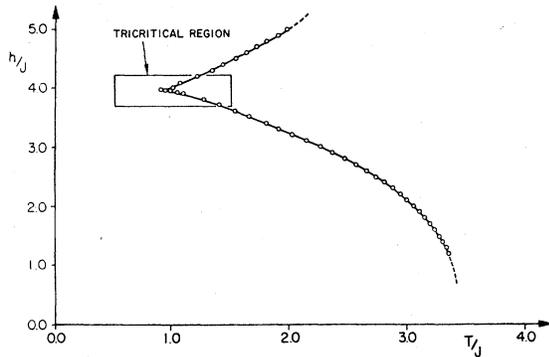


FIG. 4. Same type of data as in Fig. 3, but now  $K = J/2$ . The presumed tricritical region is shown with a rectangle.

and 5. We suggest that the upper curve of specific-heat peaks persists in the limit of large  $N$  and intersects the ultimate phase boundary at the tricritical point. It may even intersect with zero slope. The lower curve should develop into the  $\lambda$  line in the expected way. If this conjecture is correct, it provides an additional signature for the tricritical point in addition to being at the intersection of the first-order line and the  $\lambda$  line. This could be of possible value in pinning down a tricritical point experimentally with specific heat data. For example, these high-field peaks are reported in the work on dysprosium aluminum garnet (DyAlG) by Landau and coworkers,<sup>18</sup> but their relation to the tricritical point in that material is not clear. The diagrams in Figs. 4 and 5 are very similar to spin flop or bicritical phase diagrams,<sup>8</sup> although we emphasize again that the upper curve is *not* a precursor to a phase boundary, in contrast to what one would observe in an actual bicritical system.

Roughly then, within the context of our conjecture, these upper specific-heat curves are "pointing" at what eventually becomes the tricritical point. A

crude extrapolation (see below) of the data shown to  $N = \infty$  provides an estimate for the location of the tricritical point. Similar data when  $K = J$  also has been obtained. These estimates are:

$T_t/J$	$h_t/J$	$K/J$	
$1.05 \pm 0.05$	$3.98 \pm 0.01$	$\frac{1}{2}$	(4)
$2.15 \pm 0.05$	$3.96 \pm 0.01$	1	

The errors are basically subjective and rely on the topology discussed above. The outstanding characteristic of the trend of these estimates would be the extreme flatness of a smooth curve drawn from the tricritical point to  $(h/J = 4.0, T/J = 0)$ . This is possible evidence for a crossover exponent  $\phi_t$  that is quite small in two dimensions.

We have considered how the maxima in  $C_h$  on the curves in Figs. 4 and 5 grow with  $N$  for fixed  $h$ . Specifically, for the case  $K/J = \frac{1}{2}$  we have plotted (not shown)  $C_{\max}(N)$  versus various simple functions of  $N$  for the field  $h/J = 3.99$ . We tried  $N^2$ ,  $N^3$ ,  $N^4$ ,  $e^N$ , and  $e^{N^2}$ ; roughly, the best "fit" seems to be somewhere between the last two functions. That is, we see growth faster than a small power of  $N$ . What should we expect? If this value of the field were less than the tricritical field, one would expect<sup>10,17</sup> an asymptotic rise of  $\ln N$  (and it is easy to generate data consistent with this at small fields). If the field were exactly the tricritical field, one would expect a rise of  $N^{\tilde{\alpha}}$ , where finite size scaling<sup>10</sup> predicts  $\tilde{\alpha} = \alpha_t/\nu_t = 2\alpha_t/(2 - \alpha_t)$ . Thus, one has a bound, within scaling,  $\tilde{\alpha} < 2$ . Since  $C_{\max}$  is observed to increase faster than this, we conclude that this particular value of the field is larger than  $h_t/J$ , which is (barely) consistent with the estimate in Eq. (4). One may also want to interpret this fast increase as real evidence for the first-order line in the specific heats. The point of this example though is that one sees a problem, in principle, of determining the exponent  $\alpha_t$  with transfer matrix methods, if the tricrit-

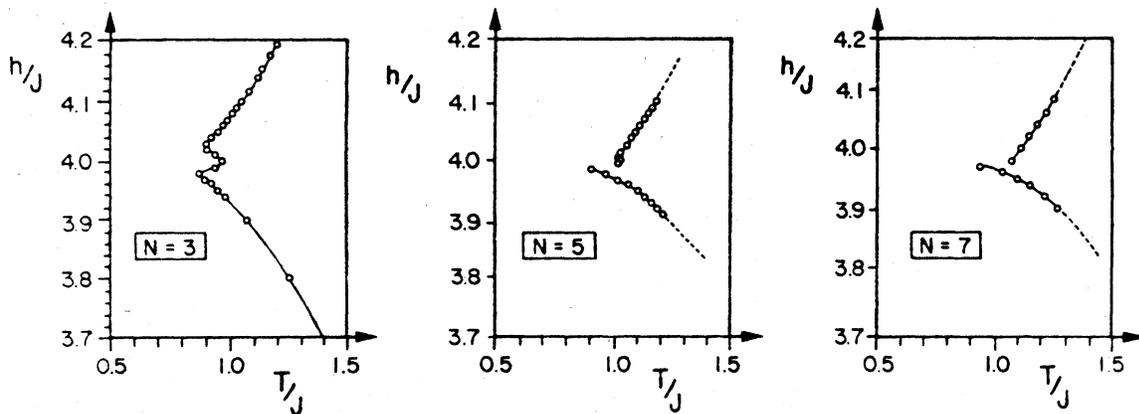


FIG. 5. Closer look at the tricritical region in Fig. 4, and additional results for  $N = 5, 7$ . Note the movement of the precursor to the  $\lambda$  line toward higher temperatures.

ical field is not known precisely.<sup>19</sup> This is because one can only hope to measure, for finite  $N$ , an effective exponent  $\tilde{\alpha}_{\text{eff}}$  in the sense of Riedel and Wegner.<sup>20</sup> If indeed  $C_{\text{max}}$  increases faster than any power of  $N$  along the first-order line, then one sees that the effective exponent varies from zero to infinity in the tricritical region! Very similar troubles seem to occur when one attempts to determine tricritical exponents via high-temperature series,<sup>21</sup> where another effective exponent ( $\gamma_t$ , usually) seems to vary through a considerable range in the tricritical region. So, we will not attempt to make tricritical exponent estimates here, due to the uncertainties in Eq. (4).

As a final application of these specific-heat data, we want to explore the possible validity of the Onsager specific-heat temperature shift<sup>9</sup>  $N^{-2} \ln N$  in our model here. Our boundary conditions are not exactly those that Onsager used,<sup>9</sup> but this should be irrelevant; the essential point is that we have an  $N \times \infty$  Ising-like system with some sort of periodicity at the edges. Shown in Fig. 6 is a plot of temperatures where the specific heat peaks,  $T_{\text{max}}(N)/J$  vs  $N^{-2} \ln N$  when  $h = 0$  and  $K/J = 1$ . We have allowed both odd and even  $N$ . Extrapolation, by drawing a straight line through the last two points, to  $N = \infty$ , yields the estimate  $T_{\infty}/J = 5.25$ , as compared with the Dalton and Wood high-temperature series estimate<sup>22</sup> of 5.260. We conclude that the  $N^{-2} \ln N$  shift is probably valid for this case. More generally, one knows from finite size scaling theory<sup>10</sup> that the leading temperature shift is predicted to be  $AN^{-1/\nu}$ ; thus it is governed by a power characteristic of the universality class. We suggest that when the amplitude  $A$  vanishes, as it does here, that the resulting power is also universal. If this is true, it would be interesting to know the relation of the exponent to other aspects of the critical behavior.

As one might expect, plots similar to Fig. 6, but for nonzero magnetic fields, exhibit considerable curvature in the tricritical region. These curved plots, together with the assumption about the curve of high-field peaks intersecting the tricritical point, provided the basis for the estimates of Eq. (4). From Eq. (4) and data for small values of  $K/J$  one has, roughly, that  $T_i \approx K$  for fixed  $J$  and small  $K$ . Moreover, the characteristic shape of Fig. 4, in contrast to Fig. 3, seems to occur for arbitrarily small  $K > 0$ , in agreement with the approximate lattice renormalization group calculations of Nienhuis and Nauenberg, and, as pointed out by them, in contrast to the result of mean-field theory.<sup>5</sup> If the asymptotic  $K = 0$  phase diagram remains like Fig. 3, then one has an abrupt jump in the slope of the phase boundary at  $h/J = 4.0$  from a negative value to zero, as  $K$  increases from zero. With the estimates of Eq. (4) in mind, and

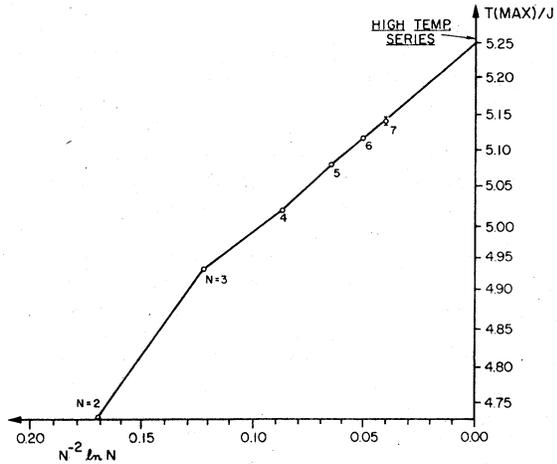


FIG. 6. Temperature at which the specific-heat peaks  $T_{\text{max}}(N)/J$  plotted vs  $N^{-2} \ln N$ , when the magnetic field  $h = 0$  and  $K = J$ . A straight line drawn between the last two points is extended to  $N = \infty$ ; an arrow indicates high-temperature series.

the behavior seen in the figures, the reader can then picture the general qualitative evolution of the phase diagram, as a function of  $K/J$  for the range  $0 \leq K/J \leq 1.0$ . This qualitative behavior seems to bear little contact with the prediction of mean-field theory.<sup>5</sup>

## V. SUMMARY

We have investigated the small- $N$  behavior of a model on  $N \times \infty$  strips of spins thought to exhibit a tricritical phase diagram in the two-dimensional limit. We have discovered that if one attempts to locate a tricritical point in real systems with specific-heat data, it may be interesting to follow a curve of specific-heat peaks at large nonordering field down into the tricritical region. We also suggested, and provided evidence for, the universality of the  $N^{-2} \ln N$  temperature shift in models where the boundary conditions make this the leading correction.

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