Finite-size scaling study of the two-dimensional Blume-Capel model

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The phase diagram of the two-dimensional Blume-Capel model is investigated by using the technique of phenomenological finite-size scaling. The location of the tricritical point and the values of the critical and tricritical exponents are determined. The location of the tricritical point ($T_t=0.610\pm0.005$, $D_t=1.9655\pm0.0010$) is well outside the error bars for the value quoted in previous Monte Carlo simulations but in excellent agreement with more recent Monte Carlo renormalization-group results. The values of the critical and tricritical exponents, with the exception of the leading thermal tricritical exponent, are in excellent agreement with previous calculations, conjectured values, and Monte Carlo renormalization-group studies.

The Blume-Capel model[1] is a spin-1 Ising model which exhibits a line of continuous phase transitions, a line of first-order phase transitions and a tricritical point. The Hamiltonian of the model is given by

$$\mathscr{H}=-J\sum_{(ij)}S_iS_j+D\sum_i S_i^2-H\sum_i S_i \ , \qquad (1)$$

where the spins (S_i) take on the values 0, ±1, and (ij) denotes nearest-neighbor pairs on a two-dimensional square lattice. The parameters J,H,D are the coupling constant, magnetic field, and crystal-field coupling, respectively. Considerable theoretical work has been applied to this model. It has been analyzed using mean-field theory,[1] real-space renormalization-group calculations,[2] Monte Carlo simulations,[3] ϵ-expansion renormalization groups,[4] high- and low-temperature series calculations,[5] and Monte Carlo renormalization-group analysis.[6] Throughout this paper the spin coupling J is set to unity and the crystal field and magnetic field are measured in units of J. The phase diagram of this model in zero magnetic field is shown in Fig. 1. For crystal-field couplings less than the tricritical value $(D<D_t)$ the system undergoes an Ising-like continuous phase transition to an ordered ferromagnetic state as the temperature is lowered. The transition line between (T_t,D_t) and (0,2) is a line of first-order phase transitions. The magnetization $(\langle S_i\rangle)$ has a jump discontinuity across the first-order phase transition line. The point (T_t,D_t) is the tricritical point which separates the first-order line from the continuous phase transition line. Early Monte Carlo simulations[3] and placed the tricritical point near $T_t=0.67, D_t=1.94$ but with rather large error bars on these values. The fact that Monte Carlo simulations have difficulty in accurately locating tricritical points is understandable[3,6] due to the exceptionally large fluctuations in the order parameter close to the tricritical point. Real-space renormalization-group studies[2] placed a tricritical point at $T_t=0.580, D_t=1.97$.

In this paper we will present a phenomenological finite-size scaling analysis[7] of this model. This technique has previously been used to analyze other models with tricritical points.[8–11] The method is known to be very reliable and accurate in its predictions of the location of tricritical points and it gives accurate predictions for the values of the leading critical exponents. The accuracy of this method allows us to pinpoint the tricritical point in this model at $T_t=0.610\pm0.005$ and $D_t=1.9655\pm0005$ which is well outside the range quoted in the Monte-Carlo-simulation work[3] for the location of the tricritical point. A more recent Monte Carlo renormalization-group calculation,[12] however, gives the location of the tricritical point as $T_t=0.6091\pm0.0030$ and $D_t=1.9655\pm0.0151$ which is in excellent agreement with this work. The critical exponents along the critical line take on values consistent with the exponents of the two-dimensional Ising model (as expected). The tricritical exponents are more slowly converged than is the case with previous finite-size scaling studies of tricritical points[8–11] but are in reasonable agreement with the expected values[6,13–16] and the values found by the most recent Monte Carlo renormalization-group calculations.[12]

The finite-size scaling technique is based on the (well founded) hypothesis[7] that the correlation length, ξ_L, in a system with a strip geometry (with strip width L) will scale near the critical line with the functional behavior

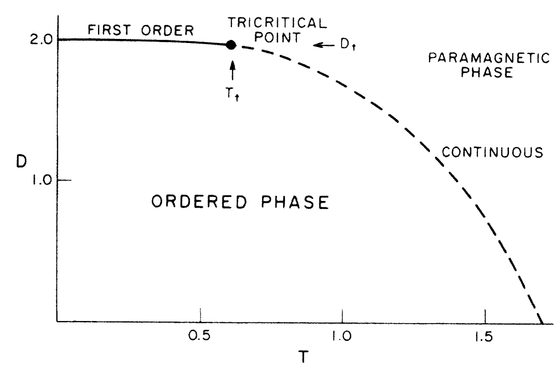

FIG. 1. Phase diagram of the Blume-Capel model. The transition line for temperatures $T>T_t$ are second order and the transition line for temperatures $T<T_t$ are first order. The point at the intersection of these two lines is the tricritical point.

$$\xi_L \approx L Q(L^{y_1} t) , \tag{2}$$

where $t=(T-T_c)/T_c$ is the dimensionless temperature deviation from the critical line. The exponent $y_1=1/\nu$ characterizes the scaling behavior of the correlation length in the infinite system as $t\to 0$ ($\xi \sim t^{-\nu}$). The phase transition line of the infinite system can be located[7] by examining the way in which the correlation length in the finite width system scales with L. At the transition line, the function ξ_L/L should be asymptotically independent of L for large L. In the disordered phase ξ_L/L will be a decreasing function of L and in the ordered phase ξ_L/L will be a sharply increasing function of L. If the functions ξ_L/L are plotted as functions of T or D for several different L's, the points where the curves cross will be finite-size scaling estimates of the critical temperature. As L increases the estimates will converge to the exact critical point. Determining whether the transition is first order or continuous involves some more analysis.[8–11] This is accomplished by examining the finite-size scaling behavior of the persistence length, $\tilde{\xi}$. The persistence length is a measure of the surface free energy between the different phases which coexist at the first-order transition line. This quantity is measured along the phase transition line (as determined by correlation length scaling). If the scaled persistence length ($\tilde{\xi}/L$) on the transition line is a decreasing function of L then the transition is continuous. If the scaled persistence length is an increasing function of L then the transition is first order. The scaled persistence length is asymtotically independent of L at the tricritical point. The scaled form of the persistence length along the transition line near the tricritical point is[11]

$$\frac{\tilde{\xi}_L^*}{L} \approx Q(L^{y_2^t} g) . \tag{3}$$

The asterisk indicates that the function is evaluated on the transition line [as determined by Eq. (2)]. The parameter g is the scaled distance from the tricritical point *along* the transition line. The parameter g is negative on the first-order line and positive on the continuous boundary. The exponent y_2^t determines the scaling of thermodynamic quantities along the transition line close to the tricritical point.[2–5,12]

The correlation length and persistence length are simple functions of the leading eigenvalues of the transfer matrix of the model. For this model the transfer matrix is a $3^L \times 3^L$ real matrix. The leading eigenvalues are found by using a treppen-iteration procedure[17] optimized to use the sparse representation of the transfer matrix.[18] The correlation length is determined by

$$\xi_L = \frac{1}{\ln(\lambda_1/\lambda_2)} \tag{4}$$

and the persistence length is given by

$$\tilde{\xi}_L = \frac{1}{\ln(\lambda_1/\lambda_3)} , \tag{5}$$

where $\lambda_1,\lambda_2,\lambda_3$ are (in decending order) the three largest eigenvalues of the transfer matrix. At a second-order transition only the leading two eigenvalues will be degenerate in the infinite L limit. However, at a first-order transition of this type all three largest eigenvalues of the transfer matrix will be degenerate in the limit $L\to\infty$ because of the existence of three coexisting phases along this line. This accounts for this particular choice for the definition of the persistence length.

The calculations were performed on a Control Data Corporation Cyber 205 supercomputer at Colorado State University. The computer code which implements the sparse-matrix treppen-iteration technique was vectorized specifically for use on this machine. About 5 central processing unit hours were used for the calculations described here. The largest strip width used ($L=10$) gave a transfer matrix with a dimension of $59\,049 \times 59\,049$.

Figure 2 shows the scaled correlation length ξ_L/L at fixed temperature, $T=0.61$, for a range of D on either side of the transition line. (This line happens to go through the tricritical point but the equivalent curves taken from elsewhere in the phase diagram display similar convergence properties.) The location of the phase transition line for this value of T, $D^*(T)$, is determined by the points where the curves cross. For example, at this value of temperature the transition is accurately located at $D^*=1.9655$. Temperature or crystal-field scans of this type were performed over the entire phase diagram in order to determine the exact location of the transition line. Once the transition line is determined, the scaled persistence length is calculated along the transition line. (Near the tricritical point and along the first-order line the persistence length peaks strongly at the transition line. It is in fact the maximum value of the persistence length for

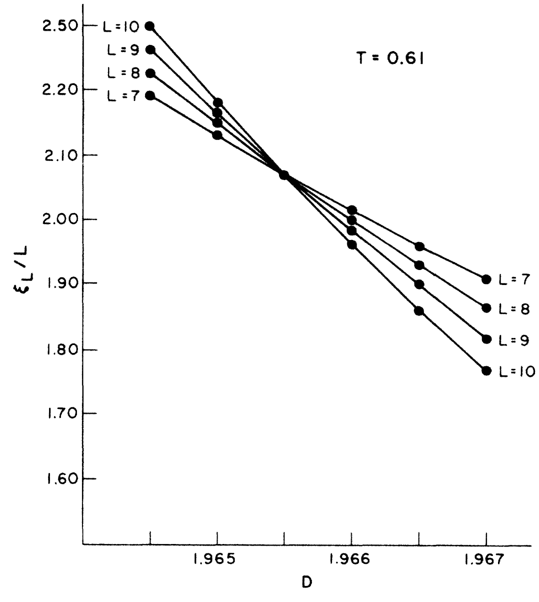

FIG. 2. Scaled correlation length plotted versus D at fixed temperature $T=0.61$. The data are shown as solid circles and the lines through the points are guides to the eye. The scaled correlation lengths cross at finite-size scaling estimates of the transition temperature. This particular set of data coincides with the tricritical point but other regions of the phase diagram show similar convergence properties.

a given temperature which was used to generate the data in Fig. 3.) Figure 3 shows the scaled persistence length along the transition line near the tricritical point. The curves are independent of L at $T=0.61$. From this data we can determine that the tricritical point is located at $T_t=0.610\pm0.005$ and $D_t=1.9655\pm0.005$. The quoted errors are a generous estimate of the uncertainty based on the finite-size scaling convergence rate. The results of the scans of the phase diagram are presented in Table I. Note the excellent agreement with the value of T_c obtained by high- and low-temperature series[5] at $D=0$ ($T_c=1.690\pm0.006$).

The scaling form of the correlation length in the neighborhood of the tricritical point is given by[8–11,18]

$$\frac{\xi_L}{L}\approx Q(L^{y_1^t}t,L^{y_2^t}g,L^{y_3^t}h)\ , \qquad (6)$$

where t is the distance from the tricritical point along the temperature scaling axis (transverse to the transition line), g is the deviation from the tricritical point, along a line tangent to the transition line at the tricritical point, and h measures the distance from the tricritical point along a direction parallel to the magnetic field axis. By closely examining the behavior of the scaling function close to the tricritical point we can determine y_1^t, y_2^t, and y_3^t. For example, the values of y_1^t and y_2^t can be determined by the scaling behavior of the effective exponent[11,19]

$$y^{\text{eff}}=\frac{\ln(|\nabla\xi_L|/|\nabla\xi_{L-1}|)}{\ln[L/(L-1)]}-1\ . \qquad (7)$$

The gradients are numerical derivatives taken in the T-D plane and evaluated at the tricritical point. The value of y^{eff} will depend on the direction in the D-T plane in which the gradients are taken. By plotting the effective exponent y^{eff} as a function of direction in the D-T plane the scaling directions and the exponents can be determined simultaneously.[11,19] The values of y^{eff} in the directions where y^{eff} is independent of L determine the exponents y_1^t and y_2^t. The exponent y_3^t is determined by varying H when $T=T_t$ and $D=D_t$. An alternative method of finding y_2^t is given by using Eq. (3), i.e.,

$$y_2^t\approx\frac{\ln\left[\dfrac{d\tilde{\xi}_L^*/dT}{d\tilde{\xi}_{L-1}^*/dT}\right]}{\ln[L/(L-1)]}\ . \qquad (8)$$

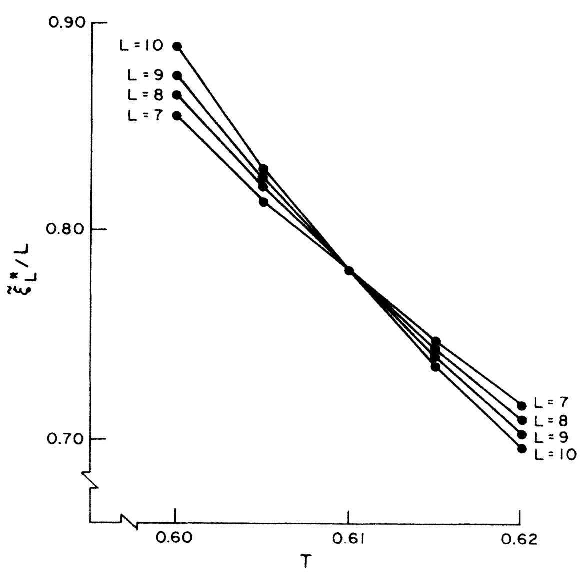

FIG. 3. Scaled persistence length along the transition line as a function of temperature near the tricritical point. The data points are shown as solid circles and the lines through the points are guides to the eye. The scaled persistence lengths cross at the finite-size scaling estimates of the tricritical temperature. The ratio of slopes of these curves at the tricritical point determines the exponent y_2^t by using Eq. (8).

TABLE I. Critical and first-order lines.

Temperature T	Crystal field D	Order of transition
1.695	0.00	second
1.567	0.50	second
1.398	1.00	second
1.150	1.50	second
0.800	1.87	second
0.700	1.92	second
0.650	1.95	second
0.620	1.962	second
0.610	1.9655	tricritical
0.600	1.969	first
0.550	1.99	first
0.500	1.992	first
0.000	2.000	first

The analysis of the scaling behavior by these methods gives the values $y_1^t=1.75\pm0.03$, $y_2^t=0.80\pm0.01$, and $y_3^t=1.90\pm0.05$. The values for y_2^t and y_3^t agree very well with the expected values[6,13–16] of $y_2^t=\frac{4}{5}$ and $y_3^t=\frac{77}{40}$. However, the leading scaling exponent, y_1^t, is significantly different from the value $y_1^t=\frac{9}{5}$ which is expected from Ising universality arguments[6,13–16] and the value $y_1^t=1.80\pm0.005$ found in recent Monte Carlo renormalization-group calculation.[12] This can be explained by noting that the temperaturelike scaling direction at the tricritical point might not lie in the D-T plane. The most general form for the nearest-neighbor version of this model involves *three* independent temperaturelike parameters and *two* magnetic fieldlike parameters. Therefore, the leading thermal scaling direction lies somewhere in this three-dimensional parameter space and not necessarily in the D-T plane. Further attempts to better determine this scaling direction in this larger parameter space using finite-size scaling techniques were unsuccessful.

The exponents along the critical line are $y_1=1.00\pm0.01$ and $y_3=1.88\pm0.02$ in agreement with universality arguments that place the Blume-Capel model in the Ising universality class ($y_1=1,y_3=\frac{15}{8}$). The exponent η which determines the algebraic decay of correlations at the critical point ($\langle S_iS_0\rangle^{T=T_c}\sim R_i^{-\eta}$ where R_i is the distance from site i to the origin) can be determined[9] by using a recent conjecture[20,21] or by using an argument based on conformal invariance.[22] These arguments predict that

$$\eta = \left[\pi \lim_{L \to \infty} \left[\frac{\xi_L^*}{L} \right] \right]^{-1} . \tag{9}$$

The asterisk indicates that the correlation length is to be evaluated at the critical point of the infinite two-dimensional system. Along the critical line we find $\eta = 0.253$ and at the tricritical point we find $\eta = 0.154$ which are both in excellent agreement with the expected values of $\eta = \frac{1}{4}$ and $\eta = \frac{3}{20}$, respectively.

In conclusion, we have performed a phenomenological finite-size scaling analysis of the two-dimensional Blume-Capel model. From this analysis we are able to accurately determine the location of the critical and first-order lines in the temperature-crystal-field plane. We are also able to locate the tricritical point accurately at $T_t = 0.61 \pm 0.005$ and $D_t = 1.9655 \pm 0.0005$. The exponents along the critical line take on the two-dimensional Ising values and the tricritical exponents, with the exception of the leading thermal exponent, are in excellent agreement with the values expected for Ising-like tricritical points. The discrepancy in the value of y_1^t is probably due to difficulty in locating the proper scaling direction in the three-dimensional parameter space.

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