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Tricritical Universality in Two Dimensions

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A powerful, new extension of the Monte Carlo renormalization-group (MCRG) method is used to accurately determine the tricritical point and exponents in two very different two-dimensional models: an Ising antiferromagnet and a Blume-Capel model. We find four relevant tricritical eigenvalues which are essentially identical for both models. We also demonstrate that subtle warning signals appear in a standard Monte Carlo calculation when a second-order transition is being misinterpreted as first order.

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The properties of many systems exhibiting simple critical points are now well known; however, models which have multicritical points are generally less well understood. The usual Monte Carlo renormalization-group (MCRG) technique[1] provides excellent critical exponent estimates but with an accuracy which is ultimately limited by the uncertainty in the critical temperature.

Numerical methods generally have extreme difficulty in finding the precise location of a multicritical point in a multidimensional space of coupling constants. To solve this problem, we have used an extension of the usual MCRG technique to calculate accurate values for tricritical couplings direct from a simulation of a system in the neighborhood of the tricritical point. This provides a determination of the tricritical point that is independent of the criteria for convergence of the eigenvalue exponents.[2]

Although the nature of tricritical behavior is now quite well known for models in three spatial dimensions,[3] the corresponding information for two-dimensional models[4-13] is scarce and sometimes contradictory. Our interest in two-dimensional tricritical behavior has been further heightened by recent developments in the study of critical behavior in two dimensions. Baxter has shown[14] that the critical exponent δ is 14 in a hard hexagon model. This discovery shows that the concept of "weak" universality[15] is not valid in two dimensions. Moreover, since there is reason to believe that this model should be in the same universality class as the three-state Potts model in two dimensions,[16] the apparent difference in the exponent δ raises significant questions. Extensive previous work[12,13,17-21] has presented a picture in which percolation, critical behavior, and tricritical behavior in a wide range of models may be viewed as different aspects of the properties of a generalized Potts model. Conjectures by den Nijs,[18] by Nienhuis, Berker, Riedel, and Schick,[12] and by Pearson[19] give explicit predictions for the continuous variation of important exponents with q for the q-state Potts model. These describe tricritical behavior as just an extension of the critical-exponent curve. The predicted deviations from "weak" universality are small along the critical portion of the fixed

line, but our study of tricritical behavior allows us to calculate the magnetic eigenvalue where the deviation from "weak" universality is great.[22]

We have studied two different two-dimensional models on a square lattice: The spin-$\frac{1}{2}$ Ising antiferromagnet with Hamiltonian

$$\mathcal{H} = J\sum_{\text{nn}} \sigma_i \sigma_j - \tfrac{1}{2}J \sum_{\text{nnn}} \sigma_i \sigma_k + H\sum_i \sigma_i, \quad (1)$$

where $\sigma_i = \pm 1$ and $J > 0$; and the spin-1 Blume-Capel ferromagnet

$$\mathcal{H} = -J\sum_{\text{nn}} \sigma_i \sigma_j - J' \sum_{\text{nnn}} \sigma_i \sigma_j + \Delta\sum_i \sigma_i{}^2, \quad (2)$$

where $J > 0$, and $\sigma_i = 0, \pm 1$. It is useful to write the generalized Hamiltonian in the form

$$H = \sum_\alpha K_\alpha S_\alpha, \quad (3)$$

where the S_α are sums of products of spin operators, and the K_α are the appropriate coupling constants with factors of $-1/kT$ absorbed.

We began by following Wilson's procedure[23] of doing Monte Carlo (MC) simulations on two different-size lattices. If the lattices have linear dimensions differing by the renormalization-group (RG) scale factor, b, one RG iteration of the larger system will make the two lattices equal in size. The differences in the correlation functions will then reflect the difference between the original and the renormalized Hamiltonians.

To determine the change in coupling constants produced by the RG transformation, we multiply the vector of correlation-function differences by the inverse of the matrix

$$\frac{\partial\langle S_\alpha{}^{(n)}\rangle}{\partial K_\beta{}^{(n)}} = \langle S_\alpha{}^{(n)} S_\beta{}^{(n)}\rangle - \langle S_\alpha{}^{(n)}\rangle\langle S_\beta{}^{(n)}\rangle. \quad (4)$$

This allows us to track the trajectory toward (or away from) the fixed point. An approximation to the fixed point can then be obtained from these changes in the coupling constants and the eigenvectors and eigenvalues of the usual MCRG analysis. By projecting back onto the space of m coupling constants included in the MC simulation, the deviations from the fixed point corresponding to the m largest eigenvalues can be eliminated. In particular, we can determine the (two) coupling constants needed to locate the tricritical point.

For direct determination of the tricritical parameters, we used a technique suggested by Wilson. The derivatives of correlation functions after n RG iterations with respect to the *original* coupling constants are given by

$$\frac{\partial\langle S_\alpha{}^{(n)}\rangle}{\partial K_\beta{}^{(0)}} = \langle S_\alpha{}^{(n)} S_\beta{}^{(0)}\rangle - \langle S_\alpha{}^{(n)}\rangle\langle S_\beta{}^{(0)}\rangle. \quad (5)$$

We can determine how the original coupling constants should be changed to make the correlation functions equal by solving the equation

$$\langle S_\alpha{}^{(n)}\rangle_L - \langle S_\alpha{}^{(n-1)}\rangle_S = \sum_\beta \left[\frac{\partial\langle S_\alpha{}^{(n)}\rangle_L}{\partial K_\beta{}^{(0)}} - \frac{\partial\langle S_\alpha{}^{(n-1)}\rangle_S}{\partial K_\beta{}^{(0)}}\right]\delta K_\beta{}^{(0)}, \quad (6)$$

where $\langle S_\alpha{}^{(n)}\rangle_L$ and $\langle S_\alpha{}^{(n-1)}\rangle_S$ are the correlation functions for the "large" and "small" lattices, respectively. As the number of RG iterations, n, increases, this procedure becomes increasingly sensitive to relevant perturbations (and *insensitive* to irrelevant perturbations), and provides an accurate, systematically improvable estimate for the critical or tricritical parameters.

The two models were examined with use of quite different RG transformations. The Ising antiferromagnet ($\sigma = \pm 1$) was studied with use of a $b = \sqrt{5}$ transformation[2,24] in which the block spins were made up of a central spin and its four next-nearest neighbors. The odd-symmetry couplings for this model are "staggered" couplings which alternate in sign between sublattices. The Blume-Capel model ($\sigma = 0, \pm 1$) was studied with use of a $b = 2$ block-spin transformation with a "plurality rule." Ties were decided with use of a random-number generator.

Using the extended MCRG technique outlined above, we were able to accurately locate the tricritical coupling of the Ising antiferromagnet $K_1 = H_t/kT_t = 3.283 \pm 0.01$ and $K_2 = -J/kT_t = -0.828 \mp 0.006$. A total of four relevant eigenvalues were found, and Table I shows the variation with iteration for three different lattice sizes. For the Blume-Capel model (which is identical to the generalized Potts model considered in Refs. 10–13), we carried the procedure one step further and first applied the method with a single RG iteration starting with a nearest-neighbor model (i.e., $J' = 0$) to also find the deviation from the fixed point in the direction of the largest irrelevant eigenvector. This allowed us to move along a line of tricritical points towards the fixed point, and improve convergence. We estimate the optimal next-nearest–neighbor coupling to be $K_2 = J'/kT_t = 0.2804$. With K_2 held fixed at this value, we found the tricritical point to be located at $K_1 = J/kT_t = 1.246 \pm 0.005$, and $K_3 = -\Delta_t/kT_t = -2.99 \mp 0.01$; the corresponding eigenvalue

TABLE I. Eigenvalue variation with iteration. Entries represent average values obtained from the analyses that use the two or three largest numbers of couplings. The number of MC steps per spin is also indicated for each lattice size.

	Antiferromagnet											
	$L = 4\sqrt{5}$				$L = 20$				$L = 20\sqrt{5}$			
Iteration	y_1^e	y_2^e	y_1^o	y_2^o	y_1^e	y_2^e	y_1^o	y_2^o	y_1^e	y_2^e	y_1^o	y_2^o
1	1.766	0.785	1.933	1.100	1.763	0.730	1.930	1.064	1.766	0.738	1.930	1.059
2					1.789	0.863	1.935	1.165	1.784	0.844	1.933	1.127
3									1.789	0.838	1.931	1.119
	9×10^4 MCS/s				9×10^4 MCS/s				5×10^4 MCS/s			
	Blume-Capel											
	$L = 8$				$L = 16$				$L = 32$			
1	1.783	0.713	1.933	1.112	1.785	0.736	1.934	1.120	1.785	0.715	1.934	1.120
2					1.796	0.777	1.933	1.125	1.799	0.795	1.934	1.137
3									1.805	0.835	1.929	1.136
	1.2×10^6 MCS/s				4.58×10^5 MCS/s				2.24×10^5 MCS/s			

flows are shown in Table I. For both models, the line of transitions could be determined more accurately than could the location of the tricritical point on this line. The quoted errors in the coupling constants are correlated, and thus cannot simultaneously assume their extremum values except in a direction approximately tangent to the phase boundary. An examination of Table I shows that for each model the eigenvalue variation with iteration is essentially the same for all three lattice sizes. Clearly, then, our results show no finite-size effects. In addition, the eigenvalue estimates are virtually identical for the two models: $y_1^e = 1.80 \pm 0.02$, $y_2^e = 0.84 \pm 0.05$; $y_1^o = 1.93 \pm 0.01$, and $y_2^o = 1.13 \pm 0.02$. The dominant source of error, at least for the estimates of the largest even and odd eigenvalues, is the small remaining uncertainty in the location of the tricritical points; statistical errors and finite-size effects are practically negligible. We again emphasize that the tricritical-point locations have been determined independent of the convergence in Table I. Our results quite accurately confirm both the predictions[12,13,18,19] for the tricritical values of $y_T = 1.80$ and $y_H = 1.925$. Our eigenvalue estimates, together with the usual scaling relations, lead to the following tricritical exponents: $\nu_t = 0.56$, $\alpha_t = 0.89$, $\delta_t = 27.6$, $\eta_t = 0.14$, $\gamma_t = 1.03$, $\beta_t = 0.039$, and the crossover exponent $\phi_t = 0.47$.

One surprising feature of these values is that several of them are quite close to the mean-field values which are exact in three dimensions. (The rapid convergence for y_1^e and y_1^o reflects the absence of logarithmic correction terms.)

The noticeable difference between our present estimate of T_t for the nnn antiferromagnet and that obtained from a standard Monte Carlo method was somewhat disturbing. To understand the source of this difficulty, we carried out additional Monte Carlo calculations just above the tricritical points in both models. Apparent hysteresis was observed, but it became narrower as the lattice size decreased. The time dependence of the properties showed large fluctuations and regions which could be interpreted as showing metastability. A very striking phenomenon is evident in the histogram for $L^{-2}\sum_i \sigma_i^2$ for the Blume-Capel model which is shown in Fig. 1. Even though the system is just above T_t, the double-peak structure would suggest a first-order transition! The only warning signal that such an identification may be spurious is a small size dependence. The peaks should continue to move together as the lattice size increases until they join to form a single peak. We again emphasize that the difficulties in locating multicritical points which appear in other numerical techniques, such as series expansions[25] or standard Monte Carlo

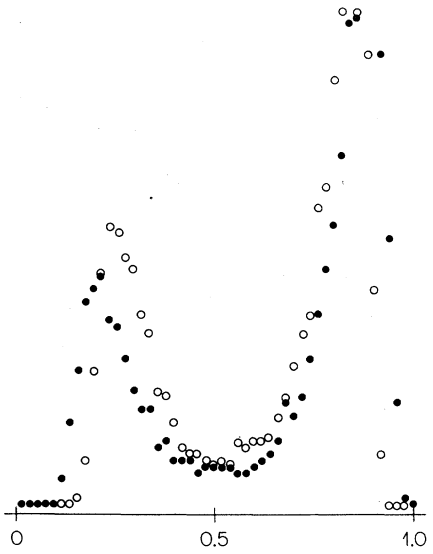

FIG. 1. Histogram for the distribution of $L^{-2}\Sigma_i \sigma_i{}^2$ during a standard Monte Carlo calculation on the Blume-Capel model with $J = 1.241$, $J' = 0.2804$, and $\Delta = -2.98$. Open circles are for $L = 32$; closed circles are for $L = 16$.

methods, can be avoided with use of the extended MCRG method.

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