Monte Carlo renormalization-group study of tricritical behavior in two dimensions

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Using a Monte Carlo renormalization-group (MCRG) method we study tricritical behavior in two very different two-dimensional spin models: the Blume-Capel ferromagnet and the next-nearestneighbor Ising antiferromagnet. The MCRG method is used to locate accurately tricritical points independent of the convergence of eigenvalue estimates. Despite the different symmetries and the different renormalization transformations used for the two models, in both cases we find four relevant tricritical eigenvalues which are essentially identical for both models. For the antiferromagnet, there is no indication of any decomposition of the tricritical point as predicted by meanfield theory, for ratios of intrasublattice to intersublattice coupling as small as $\frac{1}{8}$.

I. INTRODUCTION

Tricritical behavior¹ has been investigated in detail using mean-field theory, series expansions, renormalizationgroup theory, Monte Carlo methods, and transfer-matrix calculations. The bulk of this work has been carried out for three-dimensional models and shows that for dimensionality $d \geq 3$, the tricritical exponents are mean-fieldlike (classical) apart from logarithmic corrections for $d=3$. Mean-field theory² also predicts that for antiferromagnets in a field, tricritical points appear on the phase boundary only if the ratio of the intrasublattice to intersublattice coupling is sufficiently strong. In two dimensions, fluctuations are strong and are expected to modify the tricritical exponents and possibly even the qualitative features of the phase boundary. We have therefore carried out detailed studies of two different two-dimensional models on a square lattice in order to determine the tricritical exponents and the general dependence of the tricritical behavior on features of the model. The first model was the spin-1 Blume-Capel ferromagnet with Hamiltonian

$$
\mathcal{H} = -J \sum_{NN} s_i s_j - J' \sum_{NNN} s_i s_j + \Delta \sum_i s_i^2, \qquad (1)
$$

where J, $J' > 0$, and $s_i = 0, \pm 1$. The second model is the spin- $\frac{1}{2}$ next-nearest-neighbor (NNN) Ising antiferroma net with Hamiltonian

$$
\mathcal{H} = J \sum_{NN} \sigma_i \sigma_j - J' \sum_{NNN} \sigma_i \sigma_k - H \sum_i \sigma_i , \qquad (2)
$$

where $J, J' > 0$, $\sigma = \pm 1$, and the sums are over nearestneighbor (NN) and NNN pairs, respectively. (These Hamiltonians can conveniently be represented in terms of dimensionless coupling constants, e.g., $K_1 = -J/k_BT$, $K_2 = J'/k_B T$, $K_3 = H/k_B T$.) For the square lattice, there are four NN and four NNN pairs for each site, so the ratio of intrasublattice coupling $4J'$ to intersublattice coupling 4J is given by $R = J'/J$. According to mean-field theory, if the ratio R of intrasublattice coupling to intersublattice coupling is less than a critical value $R_c = \frac{3}{5}$, the tricritical point splits into a critical endpoint and a double critical point; thus, one of the goals of our study is to determine whether or not the tricritical point continues to be present for $R < \frac{3}{5}$. We have studied these two models using a Monte Carlo renormalization-group (MCRG) method and preliminary results have been reported elsewhere. 3 We describe the method in the next section and present our results in Sec. III. In Sec. IV we shall compare and contrast our findings with those of other studies.

II. METHOD

The basic technique used in our study was the MCRG method.⁴ We rewrite the Hamiltonian in the general form

$$
\mathcal{H} = \sum_{\alpha} K_{\alpha} S_{\alpha} \tag{3}
$$

where the S_{α} are sums of products of spin operators, and the K_{α} are the corresponding dimensionless coupling constants with factors of $-1/k_BT$ absorbed. For a particular renormalization-group (RG) transformation with scale factor b,

$$
H^{(n+1)} = R_b H^{(n)} \tag{4}
$$

Near the fixed-point Hamiltonian $H^*(K^*)$, the linearized RG transformation takes the form

$$
K_{\alpha}^{(n+1)} - K_{\alpha}^* = \sum_{\beta} T_{\alpha\beta}^*(K_{\beta}^{(n)} - K_{\beta}^*) , \qquad (5)
$$

where

$$
T_{\alpha\beta}^* = \frac{\partial K_{\alpha}^{(n+1)}}{\partial K_{\beta}^{(n)}}
$$
 (6)

and the (tri)critical properties are determined by the eigenvalues of the transformation matrix T^* in the usual way.

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C)

 \rm{c}

 \times

 1.2×10^6 MCS/s

The first requirement of the method is that the simulation to determine the tricritical exponents be performed at a tricritical point. We have determined the location of the tricritical points by following Wilson's idea⁵ of comparing the results of Monte Carlo (MC) simulations on two different-size lattices. If the ratio of the linear dimensions of the two systems is chosen to equal the scale factor b of the RG transformation, one RG iteration of the larger system will make the two lattices equal in size. Differences in the correlation functions will then be due only to differences between the original and renormalized Hamiltonians.

To determine the tricritical parameters, we used an equation which was also suggested by Wilson. $⁶$ If the</sup> original Hamiltonian were the fixed-point Hamiltonian, then the original and renormalized systems would be identical and the differences in the correlation functions would vanish. For a general initial Hamiltonian in the neighborhood of the fixed point, we can express the differences in the correlation functions by

$$
\langle S_{\alpha}^{(n)} \rangle_{L} - \langle S_{\alpha}^{(n-1)} \rangle_{S}
$$

=
$$
\sum_{\beta} \left[\frac{\partial \langle S_{\alpha}^{(n)} \rangle_{L}}{\partial K_{\beta}^{(0)}} - \frac{\partial \langle S_{\alpha}^{(n-1)} \rangle_{S}}{\partial K_{\beta}^{(0)}} \right] \delta K_{\beta}^{(0)}, \quad (7)
$$

where $\langle S_{\alpha}^{(n)} \rangle_L$ and $\langle S_{\alpha}^{(n)} \rangle_S$ are the correlation functions for the large and small lattice, respectively. Since the derivatives appearing in Eq. (7) can be expressed as

$$
\frac{\partial \langle S_{\alpha}^{(n)} \rangle_L}{\partial K_{\beta}^{(0)}} = \langle S_{\alpha}^{(n)} S_{\beta}^{(0)} \rangle - \langle S_{\alpha}^{(n)} \rangle \langle S_{\beta}^{(0)} \rangle , \qquad (8)
$$

these equations (in principle) allow the location of the fixed point to be determined.

As the number of the RG iterations increases, this procedure becomes increasingly sensitive to relevant perturbations, and increasingly insensitive to irrelevant perturbations. Thus, although it does not provide an accurate determination of the fixed point itself, it is very effective in accurately locating critical and tricritical points. We wish to point out that this procedure provides a prediction for the location of the tricritical point even if one is not at the tricritical point or even on the phase boundary. Thus, different predictions obtained using slightly different Hamiltonians can be used to estimate the error in the location of the tricritical point.

The two models were examined using quite different RG transforrnations. For the Blume-Capel model $(s=0, \pm 1)$, we used an $a, b = 2$ block-spin transformation with a "plurality rule" and ties decided with the random number generator. For the Ising antiferromagnet $(\sigma = \pm 1)$, we used a $b = \sqrt{5}$ transformation^{7,8} suggested by van Leeuwen, 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 the "staggered fields" which alternate in sign between the two sublattices.

	Lattice size (L)					
	32	16				
105 MCS/site used	13.6	18.5	6.1	11.7		
10 ⁴ MCS/site discarded	90		6	90		
MCS/site between data	20	20	20	10		
Relaxation time (MCS/site)	2100	670	190	41		

TABLE II. MC simulation data for final MCRG calculations. $(D_I=0.05664, K_{DG}=-0.82090)$. Data taken for correlation functions every 10 MCS/site.

III. RESULTS

A. 81ume-Capel model

For the study of the Blume-Capel model, we followed two different approaches. First, we applied the extended MCRG method described in Sec. II, using just a single iteration on the large lattice and starting with a NN model (i.e., $J' = 0$). From this calculation we were able to determine the deviation of the initial Hamiltonian from the fixed point in the direction of the largest irrelevant eigenvector. This procedure allowed us to move along a line of tricritical points towards the tricritical fixed point and thus improve convergence. We estimate the optimal NNN coupling to be $K_2 = J'/k_B T_t = 0.2804$. With K_2 held fixed at this value, we found the tricritical point to be located at $K_1 = J/k_B T_t = 1.246 \pm 0.005$ and K_3 $=-\Delta_t / k_B T_t = -2.99 \pm 0.01$. In terms of the parameters in the Hamiltonian given in Eq. (1), the tricritical values were $k_B T_t / J = 0.8026 \pm 0.0032$, $\Delta_t / J = 2.400 \pm 0.018$, and $J'/J=0.225$. The corresponding eigenvalues are shown in Table I.

The second calculation which we made on the 81ume-Capel model set the second-neighbor coupling $K_2=0$, in order to make a direct comparison to other theoretical predictions for the location of the tricritical point. Somewhat to our surprise, the convergence of the tricritical exponents was very nearly as good for this model as it was when second-neighbor couplings were included. We made very long MC simulations using multiple runs to get both good statistics and reliable error estimates. Table II contains information on the details of the simulations, including estimates of the correlation times for comparison with the run lengths.

We found it convenient to perform the simulation in the discrete-Gaussian (DG} representation

$$
\mathcal{H} = -K_{\text{DG}} \sum_{(i,j)} (s_i - s_j)^2 - D \sum_i s_i^2 \,. \tag{9}
$$

This form has the advantage of containing a parameter D, which is quite small, and eigenvectors tend to be more closely parallel to K_{DG} and D directions instead of a parameter K_3 , which has a small deviation from the value $2K_1$. The specific couplings used in the RG analysis are given in Table III.

The tricritical couplings were found to be The incritical couplings were found to be
 $K_{\text{DG}} = -0.8209 \pm 0.0040$ and $D = 0.0566 \pm 0.0016$. This $N_{\text{DG}} = -0.8209 \pm 0.0040$ and $D = 0.0366 \pm 0.0016$. This
would correspond to $K_1 = 1.642 \pm 0.008$ and would correspond to $K_1 = 1.642 \pm 0.008$ and
 $K_3 = -3.227 \pm 0.016$ or $k_B T_t / J = 0.6091 \pm 0.0030$ and Δ , /J = 1.9655 ± 0.0151. Using these values for the tricritical couplings, we determined the leading tricritical exponents from the simulations of lattices varying in size from 4×4 to 32×32 . The results are shown in Tables IV—IX, and they exhibit ^a remarkably weak size dependence.

The tricritical exponents for q -state Potts models were conjectured in a series of papers, and the belief that these

TABLE III. Coupling constants for the MCRG analysis of the tricritical point in the $d = 2$ Blume-Capel model. Operators are in the discrete Gaussian (DG) form [see Eq. (10)], $s_i = \pm 1, 0$. Numbers in parentheses give the relative positions of interacting pairs.

N_c	Description
	Even couplings
1	s_i^2
2	Nearest-neighbor (10) [i.e., $(s_i - s_j)^2$]
3	Next-nearest-neighbor (11)
4	Third neighbor (20)
5	Fourth neighbor (21)
6	Four-spin coupling around
	a NN plaquette, $s_i s_j s_k s_l - s_l^2$
7	Four-spin coupling on a
	next-nearest-neighbor plaquette $s_i s_j s_k s_1 - s_i^2$
8	NN biquadratic exchange (10),
	$s_i^2s_i^2$ - s_is_i
9	NNN biquadratic exchange (11),
	$s_i^2s_j^2$ - s_is_j
10	Fifth neighbor (22)
	Odd couplings
1	Magnetic field
2	s_i^2 times (10) neighbor
$\overline{\mathbf{3}}$	s_i^2 times (11) neighbor
4	Three spins on a NN plaquette,
	$(00)-(10)-(11)$
5	Three spins in a row,
	$(00)-(10)-(20)$
6	Three spins at an angle,
	$(00)-(10)-(21)$

TABLE IV. Estimated deviations of the final simulated coupling constants $(0.05664, -0.8209)$ from the true tricritical values $d = 2$ Blume-Capel model. Upper line is the calculated deviation of delta and the lower for K , for each level of renormalization. Statistical error is comparable to the magnitude of the deviations.

N_{r}	N_c	$32 - 16$	$16 - 8$	$8 - 4$	N,	N_c	32
	10	-0.0023	-0.0025	-0.0007		$\mathbf{2}$	0.65
		-0.0068	-0.0067	-0.0037		3	0.73
	10	-0.0016	-0.0017	-0.0005		4	0.73(
		-0.0042	-0.0037	-0.0016			0.72(
3	10	-0.0015	-0.0015			6	0.740
		-0.0036	-0.0031				0.74
4	10	-0.0016				8	0.75(
		-0.0043				9	0.75(
						1٨	0.75

TABLE V. Critical eigenvalue exponent y_{T1} (conjectured value is 1.800) for the $d = 2$ Blume-Capel model as a function of the number of RG iterations (N_r) , the number of coupling constants in the RG analysis (N_c) , and the linear dimension of the lattice (L) . 2 \times 2 RG block transformation. Estimates of the statistical error in the last digits are given in parentheses.

values were in fact exact was supported by a derivation of the thermal exponents, subject to certain assumptions, by Nienhuis.⁹ Our results for the leading relevant thermal eigenvalue are excellent. Both the statistical error and deviations from the "exact" values⁹ are, at most, 0.3% . As usual, the errors in the second eigenvalue are somewhat larger (about 2%), but again, the data are very consistent and the agreement with the exact value of 0.8 is excellent. For the leading magnetic eigenvalue, the data lie slightly (about 0.5%) above the conjectures value of 1.925, but the trend is towards a slow decrease of the eigenvalue exponent with further RG iterations. The origin of this effect is not clear, but in any case, the deviations are very small. The second magnetic eigenvalue is also in excellent agreement with the conjectured value of 1.125. The data indicate that there is a very small (about 1%) finite-size effect when the renormalized lattice is reduced to the di-

TABLE VII. Critical eigenvalue exponent y_{T3} for the $d = 2$ Blume-Capel model as a function of the number of RG iterations (N_r) , the number of coupling constants in the RG analysis (N_c) , and the linear dimension of the lattice (L) . 2×2 RG block transformation. Estimates of the statistical error in the last digits are given in parentheses.

			Lattice size (L)	
N_r	N_c	32	16	8
$\mathbf{1}$	3	$-2.09(6)$	$-2.11(4)$	$-2.26(6)$
	4	$-0.99(4)$	$-0.92(4)$	$-1.08(7)$
	5	$-0.75(4)$	$-0.65(4)$	$-0.52(6)$
	6	$-0.65(2)$	$-0.64(2)$	$-0.57(3)$
	7	$-0.40(3)$	$-0.50(4)$	$-0.46(3)$
	8	$-0.40(3)$	$-0.49(4)$	$-0.45(3)$
	9	$-0.40(3)$	$-0.47(4)$	$-0.43(3)$
	10	$-0.41(4)$	$-0.40(4)$	$-0.44(4)$
$\overline{2}$	3	$-2.12(7)$	$-2.18(4)$	
	4	$-1.01(3)$	$-1.16(7)$	
	5	$-0.71(5)$	$-0.61(7)$	
	6	$-0.57(3)$	$-0.55(4)$	
	7	$-0.38(3)$	$-0.46(4)$	
	8	$-0.35(3)$	$-0.39(4)$	
	9	$-0.32(3)$	$-0.30(4)$	
	10	$-0.33(3)$	$-0.33(7)$	
3	3	$-2.24(8)$		
	4	$-1.31(7)$		
	5	$-0.73(8)$		
	6	$-0.58(3)$		
	7	$-0.39(3)$		
	8	$-0.28(4)$		
	9	$-0.19(4)$		
	10	$-0.17(4)$		

mensions 4×4 , but the second iteration from the 32×32 lattice (which is only reduced to 8×8) shows agreement with the conjecture to within the statistical error of about 0.3% .

8. NNN antiferromagnet

Using the extended MCRG method outlined in the preceding section, we have studied the tricritical behavior preceding section, we have studied the firefitical defiavior
of the Ising antiferromagnet for $\frac{1}{8} \le R \le 1$. For $R = \frac{1}{2}$, we found a tricritical point for $K_3=H_t/k_BT_t$ $=3.283\pm0.010$ and $K_1=-J/k_B T_t=-0.828\pm0.006$. We wish to emphasize that the quoted errors in the coupling constants are correlated, and thus they cannot simultaneously assume their extremum values except in a direction approximately tangent to the phase boundary. A total of four relevant eigenvalues were found, and Table X shows the variations with iteration for three different lattice sizes. From a comparison of the results for different lattice sizes, we see that effects of finite size are negligible as long as the final transformed lattice has

 $L \geq 4$. For $L = 100$, we also show the third-largest even eigenvalue y_3^e because of the role which it plays¹⁰ in determining the finite-width behavior of results from transfermatrix calculations. locations of tricritical points for other values of R are shown in Table XI. The variation of T_t with R is linear over the entire range $\frac{1}{8} \le R \le 1$. (As T_t , moved to lower temperature with decreasing R , the quality of the data decreased. For this reason, we did the quality of the data decreased. For this reason, we did
not examine $R < \frac{1}{8}$.) In all cases, four relevant eigen values were found; as the results in Table XII indicate, the eigenvalues converge quickly with iteration to essentially identical values for all R.

IV. DISCUSSION

Due to the high precision of our data, we believe that the location of the tricritical point as well as the tricritical exponents for the Blume-Capel ferromagnet are extremely accurate. The exponent estimates which we obtained for the NNN antiferromagnet are of slightly lesser accuracy but are nonetheless consistent with the Blume-Capel values. It is also worthwhile to compare our results to those obtained by other means. Our results agree extremely well with the conjectures⁹ and lend support to the belief that they are in fact exact. In comparison, the most precise results obtained by other methods were those obtained using variational real-space renormalization-group methods with a variety of truncating approximations.

Burkhardt¹¹ used a position-space renormalizationgroup approach with nine interactions to look specifically at the tricritical point of the Blume-Capel model and found $k_B T_t / J = 0.580$, $\Delta_t / j = 1.972$, $y_t^e = 1.797$, $y_2^e = 0.798$, $y_1^o = 1.928$, and $y_2^o = 1.106$. Berker and Wortis¹² used a three-coupling renormalization-group approach to study a global parameter space in which the Blume-Capel model was a special case. Using an adjustable parameter (to make the Onsager critical point exact) they found $k_B T_t / J = 0.578$, $\Delta_t / J = 1.971$, $y_1^e = 1.837$, $y_2^e = 0.918$, $y_1^o = 1.930$, and $y_2^o = 0.868$. Both studies were done before any conjectures were made and, in retrospect, were remarkably good, although uncontrolled. Burkhardt's exponents agree with ours to better than 1%, but his estimate for the tricritical temperature is almost 5% too low. Variational RG calculations⁹ for q -state Potts lattice-gas models gave very good estimates for the tricritical exponents for $q = 2$ (i.e., the Ising model). A recent MC study of interface behavior¹³ in the twodimensional Blume-Capel model apparently overestimated the tricritical temperature as did very early MC studies of the bulk properties.¹⁴ We also showed previously³ that for a finite lattice a double peaked distribution function could be observed even on the second-order portion of the phase boundary just above T_t . (The two peaks merged only slowly as the lattice size was increased.) Early MC studies¹⁵ of the NNN antiferromagnet also overestimated the tricritical temperature. Therefore, it appears to be quite difficult to accurately locate tricritical points in two dimensions using simple MC techniques; careful finite-size analyses for a large range of lattice sizes are essential for

TABLE IX. Critical eigenvalue exponent y_{H2} for the $d = 2$ Blume-Capel model as a function of the number of RG iterations (N_r) , the number of coupling constants in the RG analysis (N_c) , and the linear dimension of the lattice (L) . 2×2 RG block transformation. Estimates of the statistical error in the last digits are given in parentheses.

TABLE X. Eigenvalue variation with iteration for the NNN antiferromagnet with $R = \frac{1}{2}$. Entries represent average values obtained from the analyses which used the two or three largest number of couplings.

					Antiferromagnet				
			$L = 4\sqrt{5}$		$L = 20$				
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	
1	1.766	0.785	1.933	1.100	1.763	0.730	1.930	1.064	
$\overline{2}$					1.789	0.863	1.935	1.165	
3									
4									
			9×10^4 MCS/s				9×10^4 MCS/s		
					Antiferromagnet				
			$L = 20\sqrt{5}$				$L = 100$		
Iteration	y_1^e	y_2^e	yî	y_2^o	y_1^e	y_2^e	y_3^e	y_1^o	y_1^o -
1	1.766	0.732	1.930	1.058	1.769	0.753	-0.43	1.931	1.076
2	1.785	0.816	1.933	1.128	1.785	0.820	-0.43	1.932	1.115
3	1.795	0.854	1.932	1.152	1.793	0.812	-0.41	1.931	1.146
4					1.795	0.877	-0.3	1.920	1.208
			4×10^5 MCS/s				5×10^4 MCS		

TABLE XI. Variation of tricritical point parameters with R.

R	$K_{\mathcal{I}}$	K_1		K_1R	
	1.628 ± 0.005	-0.415 ± 0.003	1.628 ± 0.005	-0.415 ± 0.003	
$rac{1}{2}$	3.283 ± 0.010	-0.828 ± 0.006	1.642 ± 0.005	-0.414 ± 0.003	
$rac{1}{4}$	6.583 ± 0.024	-1.653 ± 0.015	1.646 ± 0.006	-0.413 ± 0.004	
$\frac{1}{8}$	13.20 ± 0.08	-3.308 ± 0.033	1.650 ± 0.010	-0.414 ± 0.008	

TABLE XII. Eigenvalue variation with iteration for the NNN antiferromagnet with different values of R. Entries represent average values obtained from the analyses that use the two or three largest number of couplings.

	$R=1$			$R = \frac{1}{4}$			$R=\frac{1}{r}$					
Iteration	บเ็	y_2^{ϵ}	νî	v?	νĩ	v,	ν ^o	y?	νí	y5	νî	v_{2}
	1.763	0.795	1.929	1.030	1.766	0.722	1.931	1.056	1.766	0.762	1.929	1.079
$\mathbf{2}$	1.777	0.818	1.932	1.114	1.784	0.772	1.934	1.090	1.785	0.819	1.932	1.148
3	1.787	0.838	1.934	1.163	1.792	0.853	1.934	1.146	1.791	0.861	1.928	1.151

obtaining an accurate estimate.¹⁶ Other approaches to this problem have been much less accurate.¹⁷

Our estimates for the eigenvalues for the NNN antiferromagnet are essentially the same (although less precise) than those for the Blume-Capel model. The largest thermal eigenvalue, as well as the location of the tricritical point, have also been determined from finite-stripwidth transfer-matrix calculations; $18-20$ the eigenvalue estimates agree quite well with ours, although the values of y_3 , which can be extracted from the dependence of the strip width, are of the order -1.0 to -1.5 and are hence much larger in magnitude than ours. Our result appears to be consistent with the estimate for y_3 obtained for the Blume-Capel model in Table VII.²¹ Our results for the NNN antiferromagnet show no decomposition of the tri-
critical point down to a coupling $R = \frac{1}{8}$. Herrmann,¹⁹ on the other hand, examined this model with a transfermatrix finite-strip-scaling method and concluded that no tricritical point existed for $R = \frac{1}{50}$. As shown in Table XI, our data follow a linear dependence of T_t with R and predict, therefore, that for $R = \frac{1}{50}$, $k_B T_t / J \approx 0.048$. In contrast, Herrmann¹⁹ located an Ising-like critical point at $kT/J \approx 0.166$. This temperature is so high that we conjecture that, due possibly to the small strip width, he has merely located a point on the second-order line. A combination of MC and MCRG calculations²² suggests that a decomposition of the tricritical point does occur in three dimensions but only for smaller values of R than are predicted by mean-field theory. We conjecture that the increased fiuctuations in two dimensions suppress this behavior completely.

V. CONCLUSIONS

We have demonstrated how the MCRG method can be used to systematically and accurately locate a tricritical point in a two-dimensional parameter space. This procedure is of course readily extended to a higherdimensional interaction space. Very long runs have enables us to locate the tricritical point and determine the tricrical exponents with very high precision for the Blume-Capel model. We have verified the so-called exact conjectures. Our results for the NNN antiferromagnet suggest that the qualitative nature of the variation in tricritical behavior with competing couplings is not ihe same as predicted by mean-field theory, presumably due to fluctuations.

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