PHYSICAL REVIEW B VOLUME 11, NUMBER 7 1 APRIL 1975

COMMENTS AND ADDENDA

The Comments and Addenda section is for short communications which are not of such urgency as to justify publication in Physical Review Letters and are not appropriate for regular Articles. It includes only the following types of communications: (1) comments on papers previously published in The Physical Review or Physical Review Letters; (2) addenda to papers previously published in The Physical Review or Physical Review Letters, in which the additional information can be presented without the need for writing a complete article. Manuscripts intended for this section may be accompanied by a brief abstract for information-retrieval purposes. Accepted manuscripts will follow the same publication schedule as articles in this journal, and galleys will be sent to authors.

Tricritical behavior of the Ising antiferromagnet with next-nearest-neighbor ferromagnetic interactions: Mean-field-like tricritical exponents?*

Michael Wortis

Physics Department, University of Illinois, Urbana, Illinois 61801

Fredric Harbus†

Institute for Fundamental Studies,

Department of Physics and Astronomy, University of Rochester, Rochester, New York 14627

H. Eugene Stanley

Physics Department, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139

(Received 2 December 1974)

The tricritical behavior of a model studied by Harbus and Stanley is reanalyzed. The Harbus-Stanley analysis of the direct susceptibility suggested anomalous (i.e., non-mean-field-like) tricritical exponents. The tricritical point cannot be unambiguously located by present series data. We point out that, if the true tricritical temperature were actually somewhat lower than the Harbus-Stanley value, then standard ratio analysis would give tricritical exponents consistent with the Gaussian-tricritical-fixed-point analysis of Riedel and Wegner. However, the present situation remains inconclusive.

I. INTRODUCTION

The theoretical work of Bausch[1] and Riedel and Wegner[2] predicts that true and mean-field tricritical behavior[3] in three space dimensions ($d=3$) should differ at most by logarithmic corrections. Experimental work[4] on He^3-He^4 mixtures confirms this prediction. Evidence from other experimental data is at present inconclusive,[5] so there has been an active interest in the numerical study of three-dimensional lattice models by series-expansion and Monte Carlo techniques. Recent work on the $d=3$ Blume-Capel model[6,7] and the layered metamagnet[8,9] finds mean-field-like tricritical exponents. On the other hand, Harbus and Stanley[10] studied a simple-cubic $s=\frac{1}{2}$ Ising model with nearest-neighbor (nn) and next-nearest-neighbor (nnn) exchange interactions,

$$\mathcal{H}=-J_1\sum_{\langle ij\rangle}^{\mathrm{nn}} s_i s_j - J_2\sum_{\langle ij\rangle}^{\mathrm{nnn}} s_i s_j - \mu H\sum_i s_i\,, \tag{1}$$

where $s_i=\pm 1$ on each lattice site i and $J_1=-1$ (antiferromagnetic), but $J_2=\frac{1}{2}$ (ferromagnetic). The μH term represents the interaction with an external magnetic field H. The behavior is antiferromagnetic at $H=0$ but Harbus and Stanley found a tricritical point (TCP) at

$$h_t\equiv \mu H_t/k_B T_t = 0.84\pm 0.02 \quad \text{with } k_B T_t = 6.4\pm 0.1 \tag{2}$$

and characterized by a tricritical exponent[11] for the direct susceptibility

$$\gamma_t = 0.25\pm 0.05 \tag{3a}$$

distinctly different from the mean-field-like value $\gamma_t=\frac{1}{2}$. In a Monte Carlo study of the same model but with $J_2/J_1=-\frac{1}{4}$ Landau[12] finds the more uncertain value $\gamma_t=0.29\pm 0.18$. Harbus and Stanley[10] derived series for χ_{st} but did not quote a numerical value for $(\gamma_{st})_t$. We find by ratio methods that

$$(\gamma_{st})_t = 1.11\pm 0.02\ , \tag{3b}$$

where the confidence limits reflect the consistency of the Neville tables at $h=0.84$ and $k_BT=6.42$. The corresponding mean-field prediction is $(\gamma_{st})_t=1$.

This apparently dramatic departure from mean-field tricritical behavior has prompted a good deal of speculation and several thus far fruitless searches for non-Gaussian tricritical fixed points in $d=3$. In this note we point out that there is some evidence that the exponents (3) are actually spurious and that the series data in fact support mean-field tricritical exponents. The case, as we shall argue, rests on the possibility that (2) misidentifies the TCP. No final determination can be made on the basis of existing high-temperature series alone.[13]

II. DISCUSSION

The choice of TCP is crucial, if one is to obtain correct values for the tricritical exponents: The exponents γ_{st} and γ, which have Ising-like values ($\gamma_{st}=\frac{5}{4}$, $\gamma=\frac{1}{8}$) throughout the second-order region, presumably cross over discontinuously to their tricritical values, as the TCP is attained from the second-order side. Analysis of *finite* series expansions (as in Ref. 10) represents this crossover as an apparently smooth but more or less rapid decrease[14] of γ_{st} and increase of γ in the tricritical region. The TCP occurs in this region of rapid change of "effective exponents,"[15] so a small error in locating the TCP can lead to a large error in estimating tricritical exponents.

In Ref. 10 the high-temperature phase boundary[16] was located by standard methods from the well-converged series for χ_{st}. The position of the TCP along this phase boundary was then identified in two steps: (a) An eyeball sketch of the first-order phase boundary intersecting the $T=0$ axis at $\mu H=6$ (exact) joins smoothly[17] onto the second-order phase boundary at $k_B T_t \simeq 6\pm 1$. (b) Harbus and Stanley[10] then argue that the χ series, which are rather poorly converged (relative to χ_{st}) in the second-order region (where presumably $\gamma=\alpha=\frac{1}{8}$ by universality), should converge well near the TCP, where the nonordering fluctuations become large. They examine the Padé approximants to $(\chi)^p$ for a variety of values of p and h. They find Padés[18] for $p=1/\gamma=4$, $h_t=0.84$, which are strikingly more convergent than for nearby values and *exhibit a $k_B T_t$ in agreement with that obtained from* χ_{st}. On this basis they infer (2) and (3). The argument, though plausible, is open to question, particularly at step (b), as we shall discuss below.

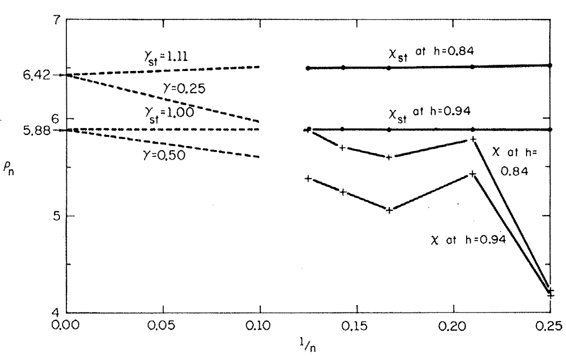

FIG. 1. Ratio plots of χ_{st} and χ at $h=0.84$ and 0.94. Series data are taken from Ref. 21. In the asymptotic region the ratios ρ_n should behave as $\rho_n=k_BT_c[1+(\theta-1)/n]$, where θ is the critical index. The straight dashed lines show the asymptotes corresponding to the exponents (3) and (5). Note that the χ_{st} series are well converged at $n=8$, while the χ series are still irregular.

TABLE I. Neville tables for k_BT_c from χ_{st}. $l_n^{(0)}=\rho_n=b_n/b_{n-1}$. The coefficients b_n are from Ref. 21. The extrapolants are derived from $l_n^{(p)}=(1/p)[nl_n^{(p-1)}-(n-p)\,l_{n-1}^{(p-1)}]$.

n	ρ_n	$l_n^{(1)}$	$l_n^{(2)}$	$l_n^{(3)}$
		$h=0.84$, $k_BT_c=6.42\pm0.03$		
5	6.515	6.468		
6	6.506	6.462	6.448	
7	6.499	6.456	6.443	6.436
8	6.493	6.450	6.430	6.409
		$h=0.94$, $k_BT_c=5.88\pm0.02$		
5	5.878	5.885		
6	5.880	5.890	5.900	
7	5.881	5.887	5.879	5.852
8	5.881	5.882	5.865	5.843

Our central observation is that, *if the TCP were located at*

$$h_t=0.94\pm0.02 \text{ (with } k_BT_t=5.88\pm0.02), \tag{4}$$

then the tricritical exponents would take on mean-field-like values to within uncertainties,[19]

$$(\gamma_{st})_t=1.00\pm0.01,\quad \gamma_t\simeq 0.4\text{–}0.6. \tag{5}$$

The location (4) is only slightly outside the Harbus-Stanley phase boundary[16] and compatible with a "reasonable" sketch [step (a)] of the first-order phase boundary.[17] The only *direct* evidence in favor of this choice is the most recent Monte Carlo data,[20] which give

$$h_t=0.92\pm0.02 \text{ (with } k_BT_t=6.0\pm0.1). \tag{6}$$

The data of Eqs. (4) and (5) are derived from standard ratio analysis of the series[21] for χ_{st} and χ. Figure 1 shows ratio plots at $h=0.84$ and 0.94. The χ_{st} series are very well converged, and we take k_BT_c from the Neville extrapolations[22] given in Table I. The exponent estimates,

$$(\gamma_{st})_n=n\left(\frac{\rho_n}{k_BT_c}-1\right)+1, \tag{7}$$

biased with these values of k_BT_c lead to the γ_{st} values quoted in (3) and (5). The ratio series for χ, on the other hand, are still noticeably irregular at $n=8$ but *must go to the same* k_BT_c. Successive

TABLE II. Padé tables for the leading singularity of χ^p.

D \ N	2	3	4	5	6
			χ^4 at $h=0.84$		
2	5.91	6.89	6.57	6.35	6.42
3	6.37	6.39	6.38	6.39	
4	6.39	6.38	6.39		
5	6.38	6.39			
6	6.39				
			χ^2 at $h=0.94$		
D \ N	2	3	4	5	6
2	4.77	5.94	5.48	5.43	5.59
3	5.18	5.46	5.43	5.47	
4	5.18	5.55	5.78		
5	4.91	5.70			
6	5.35				

estimates (7) for $(\gamma)_n$, $n=6$, 7, 8, are ($h=0.84$) 0.22, 0.20, and 0.31 and ($h=0.94$) 0.16, 0.24, and 0.33. Extrapolation is clearly not meaningful; however, the data for $h=0.94$ are certainly not *in*compatible with $\gamma=0.5$.

The Harbus-Stanley analysis of χ (applied at $h=0.94$) does not corroborate these ratio results. Table II exhibits a Padé table of the singularities of χ^2. It is strikingly less regular than the analogous table[23] for χ^4 at $h=0.84$, shown for comparison, and tends to favor a value of k_BT_c somewhat below (4). This discrepancy is not understood. If one wishes to discount the Padé evidence, one can argue that the k_BT_c values from χ and χ_{st} should only be expected to agree, *if* the corresponding (finite) series are equally well converged. It is evident from Fig. 1 that this is not the case, and, in fact, it is well known[24] that specific-heat-like series are quite generally more poorly behaved than corresponding strongly divergent susceptibility series. This reasoning, however, fails to explain why the Padés to χ^4 at $h=0.84$ are apparently so *very* well behaved. Furthermore, these same Padé methods [see discussion above (4)] were applied to the layered metamagnet[9] and in that case gave results with excellent internal consistency and in agreement with Monte Carlo analysis.[8]

In short, the present situation is not without ambiguity. A more definitive determination of the tricritical behavior of the model (1) must await better data. One possibility is the derivation of longer series, both high- and low-temperature.[13] Such work is now reported to be in progress.[25] In the interim, extant data cannot be regarded as inconsistent with mean-field-like tricritical exponents.

ACKNOWLEDGMENTS

The initial impetus for these remarks was the encouragement of Dr. M. Blume. One of us (MW) wishes to thank the Physics Departments of the Brookhaven National Laboratory and the University of Washington, Seattle, for their kind hospitality. We are grateful to Dr. D. P. Landau for unpublished Monte Carlo data and helpful comments on the manuscript. We are indebted to Dr. Chikao Kawabata, who kindly checked certain of the calculations.

*Research supported in part by the National Science Foundation, the Office of Naval Research, and the Air Force Office of Scientific Research.

†Present address: Bell Laboratories, Murray Hill, N. J. 07974.

[1]R. Bausch, Z. Phys. 254, 81 (1972).

[2]E. K. Riedel and F. J. Wegner, Phys. Rev. Lett. 29, 349 (1972); F. J. Wegner and E. K. Riedel, Phys. Rev. B 7, 248 (1973).

[3]We discuss an unconstrained system. It was recently shown by O. Entin-Wohlman, D. J. Bergman, and Y. Imry [J. Phys. C 7, 496 (1974)] that certain constrained systems exhibit tricritical behavior with non-mean-field exponents.

[4]G. Ahlers, in *The Physics of Liquid and Solid Helium*, edited by J. B. Ketterson and K. H. Bennemann (Wiley, New York, 1974), Chap. 8, contains many references.

[5]R. J. Birgeneau, G. Shirane, M. Blume, and W. C. Koehler, Phys. Rev. Lett. 33, 1098 (1974). See also Proceedings of the Conference on Critical Phenomena in Multicomponent Systems, Athens, Ga., April, 1974 (unpublished).

[6]D. M. Saul, Michael Wortis, and D. Stauffer, Phys. Rev. B 9, 4964 (1974).

[7]D. P. Landau and A. K. Jain (unpublished).

[8]B. L. Arora and D. P. Landau, AIP Conf. Proc. 10, 870 (1973).

[9]F. Harbus and H. E. Stanley, Phys. Rev. Lett. 28, 675 (1972); Phys. Rev. B 8, 1141 (1973).

[10]F. Harbus and H. E. Stanley, Phys. Rev. B 8, 1156 (1973).

[11]γ is the nonordering (ferromagnetic) susceptibility exponent, $\chi=\partial M/\partial H\sim t^{-\gamma}$ (denoted λ in Ref. 2). γ_{st} is the ordering (antiferromagnetic) susceptibility exponent, $\chi_{st}=\partial M_s/\partial H_s\sim t^{-\gamma_{st}}$ (denoted γ in Ref. 2).

[12]D. P. Landau, Phys. Rev. Lett. 28, 449 (1972).

[13]Additional *low-temperature* series would allow determination of the first-order phase boundaries by the methods of Ref. 6; however, both high- and low-temperature series must be quite long for this method to be accurate.

[14]Reference 10, Table III.

[15]E. K. Riedel and F. Wegner, Phys. Rev. B 9, 294 (1974).

[16]Reference 10, Fig. 4.

[17]It is not hard to derive several terms in the expansion of the first-order phase boundary at low temperatures: $\mu H = 6 - \frac{1}{2} k_B T_c^{-12/k_BT} + \ldots$. These suggest that the phase

boundary as T increases from zero is actually *above* the curve sketched by Harbus and Stanley, at least initially. On the other hand, there is no *a priori* reason to assume (as is done in Ref. 10) that the phase boundary is always convex upwards. Indeed, data for the Blume-Capel model, both mean-field [M. Blume, V. J. Emery, and R. B. Griffiths, Phys. Rev. A 4, 1071 (1971)] and numerical (Ref. 6), show a concave region just on the first-order side of the TCP.

[18]Reference 10, Tables VIII–X.

[19]The value (5) of $(\gamma_{st})_t$ is from standard ratio (Neville) analysis. Uncertainty quoted does not reflect uncertainty in the location of the TCP. Determination of γ_t is very crude (see Fig. 1) and (5) represents merely a range of "reasonable" possibilities. The only statement that can be made with confidence is that, if (i) the TCP is located at (4) and (ii) the χ ratios (Fig. 1) beyond order eight follow the upward trend of orders six through eight, then γ_t is certainly no lower than 0.33; i.e., it is bounded away from the Harbus-Stanley estimate $\gamma_t = 0.25$.

[20]D. P. Landau (unpublished). Footnote 4 of Ref. 11 appears to have been based on a misunderstanding. We also comment that, despite the good agreement of (4) and (6), the best Monte Carlo exponents for this model do *not* at present seem compatible with the Riedel-Wegner predictions (Ref. 2). Similar Monte Carlo calculations (Ref. 7) for the fcc Blume-Capel exponents *do* agree with Ref. 2 and the series results (Ref. 6).

[21]Reference 10, Table I.

[22]D. R. Hartree, *Numerical Analysis* (Oxford U.P., London, 1952).

[23]Reference 10, Table VIII.

[24]M. E. Fisher, Rep. Prog. Phys. 30, 615 (1967).

[25]H. E. Stanley (private communication).