Critical Behavior of the Ising, *XY*, and Heisenberg Ferromagnets on the *B*-Site Spinel Lattice*

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The critical properties of the Ising and the classical *XY* and Heisenberg ferromagnets on the *B*-site spinel lattice are studied by the method of exact high-temperature series expansions. Eight terms are obtained for each model in the susceptibility and second-moment series. Analysis of these series shows that the anomalies in the critical indices reported by Stanley and Kaplan using only six terms disappear with the use of longer series.

THE development of scaling theories[1] of critical phenomena has resulted in some understanding of what critical exponents to expect, given the dimensionality of the thermodynamic system and the nature of the ordering parameter. There are, however, certain small discrepancies between the predictions of the scaling laws and the values of critical indices determined by exact series-expansion methods; in particular, the work of Fisher and Burford,[2] on the effective correlation length index ν_1 for the Ising model, revealed a discrepancy of 2–3% between their value of ν_1 and the value predicted by the scaling relation, $3\nu_1=2-\alpha$, with[3] $\alpha=\frac{1}{8}$. Also, there are some results which are hard to understand on the basis of the arguments used in deriving the scaling laws. These include the small, but probably significant, differences between the measured critical indices of various liquid-gas systems[4] and those predicted for the Ising model. There is an unexplained discrepancy between the values obtained for the $S=\infty$ Heisenberg ferromagnet,[5] for which $\gamma\approx1.38$, and the value for the $S=\frac{1}{2}$ ferromagnet,[6] for which $\gamma\approx1.43$.

One prediction of the scaling hypothesis for lattice models is the independence of the critical indices on the lattice type. But if the scaling laws are really only correct to within a few percent, then one might expect to see a slight departure from this prediction. Some recent measurements are not inconsistent with this view,[7] but there is a large amount of evidence[2] from exact series-expansion methods to support the hypothesis of the independence of critical exponents on lattice type, at least for lattices with cubic symmetry. Very little work has been done on lattices without cubic symmetry. However, Stanley and Kaplan, and Baltzer *et al.*,[8] have found the first six terms in the susceptibility series for the Heisenberg ferromagnet on the spinel structure, using a formula of Rushbrooke and Wood,[9] on the basis of which Stanley and Kaplan surmised[10] that $\gamma\approx1.0$. This is completely at variance with the predictions, from the same number of terms, of $\gamma\approx$ 1.33–1.4 for the lattices with cubic symmetry.[11]

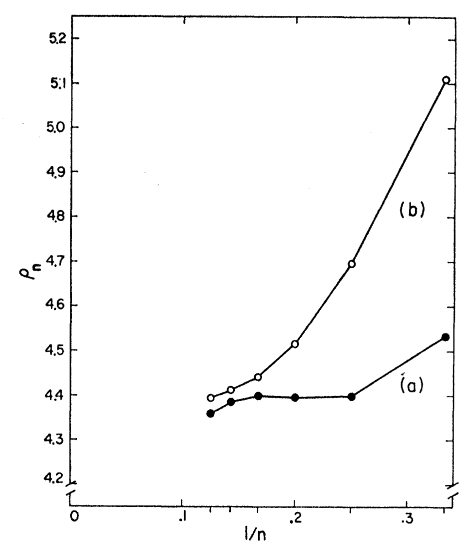

FIG. 1. Ratio of coefficients of the high-temperature series expansion of (a) the susceptibility a_n/a_{n-1} and (b) the ratio c_n/c_{n-1} for the Ising model.

Interest in the spinel structure was spurred by the discovery of the insulating ferromagnets,[12] $CdCr_2S_4$, $CdCr_2Se_4$, and $HgCr_2Se_4$. One very approximate model for these systems is that of an array of spins located on

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[9] G. S. Rushbrooke and P. J. Wood, Mol. Phys. **1**, 257 (1958).
[10] Using a Padé-approximant analysis, S. Freeman and P. J. Wojtowicz, Phys. Letters **26A**, 231 (1968), concluded that $\gamma\approx1.2$–1.3. Where ratio methods can be used (as here), they are usually more reliable and their use is more easily justified.
[11] W. Marshall, J. Gammel, and L. Morgan, Proc. Roy. Soc. (London) **275A**, 257 (1963).
[12] P. K. Baltzer, H. W. Lehmann, and M. Robbins, Phys. Rev. Letters **15**, 493 (1965); N. Menyuk, K. Dwight, R. J. Arnott, and A. Wold, J. Appl. Phys. **37**, 1387 (1966).

TABLE I. The coefficients a_n for the susceptibility χ^{zz} of the Ising and Heisenberg models and the susceptibility χ^{xx} of the XY model with the coefficients b_n for the corresponding second-moment series.

Model	Ising		XY		Heisenberg	
n	a_n	b_n	a_n	b_n	a_n	b_n
0	1		0.333333		0.333333	
1	6	6	0.666667	0.666667	0.666667	0.666667
2	30	72	1.155555	2.666667	1.111111	2.666667
3	136	580	1.860741	7.312593	1.659259	7.140741
4	598	3 864	2.895802	16.829630	2.355555	15.703704
5	2 628.8	23 088.8	4.441440	34.975648	3.304974	30.699212
6	11 565.3333	128 971.2	6.767252	68.057257	4.645612	55.669151
7	50 708.8762	688 926.4762	10.268430	126.569566	6.522448	96.040300
8	220 989.6952	3 565 320.2286	15.516152	227.810092	9.084801	160.029666

the B sites of a spinel lattice and interacting via equal nearest-neighbor exchange forces J, and this was the model used by Stanley and Kaplan.[13] In the case of the $S=\infty$ Heisenberg model, we have extended their series from six to eight terms and also obtained for the first time the first eight terms in the second-moment series. We have also studied the $S=\frac{1}{2}$ Ising model and the $S=\infty$ XY model on the same structure,[14] and found the same qualitative behavior. Namely, that with only six terms in the series a value $\gamma\approx1.0$ seems reasonable, but that on extending the series to eight terms, larger values of γ appear more likely.

The method used for obtaining the series expansion was to first derive a series expansion in $v(=J/kT)$ for the spin-spin correlation function,

$$\mathfrak{M}^{ij}(1,2)=\langle S^i(1)S^j(2)\rangle-\langle S^i(1)\rangle\langle S^j(2)\rangle, \quad (1)$$

in zero field, between arbitrary lattice sites 1 and 2 through order v^8. i and j are labels for the Cartesian components of the spin. In the calculations, we used the linked-cluster expansion developed for the Ising model by Englert.[15] Once $\mathfrak{M}^{ij}(1,2)$ is known, susceptibility and second-moment series are formed:

$$\chi^{ij}=\sum_2 \mathfrak{M}^{ij}(1,2)=\sum_n a_n v^n, \quad (2)$$

$$\mu_2{}^{ij}=\sum_2 |\mathbf{r}_1-\mathbf{r}_2|^2\mathfrak{M}^{ij}(1,2)=\sum_n b_n v^n. \quad (3)$$

χ^{ij} is the linear response of the ith component of the magnetization per site to a homogeneous magnetic field in the jth direction, and $\mu_2{}^{ij}$ is a measure of the range of correlation.[2] In Table I, we give the coefficients a_n and b_n for the three models considered. For the Ising and Heisenberg models, the coefficients refer to χ^{zz} and $\mu_2{}^{zz}$, which are the ordinary dimensionless susceptibility and second-moment series. For the XY model, they refer to χ^{xx} and $\mu_2{}^{xx}$, as these are the quantities of interest.[16] Near the Curie point χ and μ_2 are expected to diverge as

$$\chi\sim(v_c-v)^{-\gamma}, \qquad \mu_2\sim(v_c-v)^{-\gamma-2\nu_1}. \quad (4)$$

If one divides the second-moment series by the susceptibility series, one obtains a new set of coefficients c_n which are the terms in the expansion of a series which diverges as $2\nu_1$. Figure 1 shows an attempt to obtain γ and $2\nu_1$ by making a conventional ratio[17] plot of the coefficients a_n and c_n for the Ising model. Notice that for the susceptibility [curve (a) of Fig. 1], the slope of the curve, which asymptotically is a measure of $\gamma-1$, is nearly zero at $n=6$, implying $\gamma\approx1.0$, but that the later terms indicate a larger value of γ.[18] It is clear that the six-term series is not showing asymptotic behavior, and there is no reason to believe that the customary value[17] of γ will not be recovered when enough terms are available. Very similar behavior is seen in the other models; however, the Ising model exhibits the effect most dramatically. We hesitate to make definite statements about γ, ν_1, or v_c, even with eight terms.

The low value of γ obtained with only six terms on the spinel is probably connected with its four sublattice structure, little of which is "sampled" in the first six terms of the expansions. Series-expansion methods cannot be expected to be reliable until enough terms are enumerated to sample the lattice complexity. Too short series are of course an ever present danger in the exact series-expansion method of obtaining critical exponents, and may well be the cause of the other discrepancies noted.

[13] For a discussion of the exchange interactions necessary to characterize some normal cubic spinels, see K. Dwight and N. Menyuk, Phys. Rev. **163**, 435 (1967). Stanley and Kaplan, Ref. 8, considered $S=\frac{3}{2}$ corresponding to the spin-only moment of the chromium ion.

[14] The results for lattices of cubic symmetry will be published elsewhere. For these lattices the classical XY model gives $\gamma\approx1.32$, $\nu_1\approx0.67$.

[15] F. Englert, Phys. Rev. **129**, 567 (1963); D. Jasnow, M. A. Moore and M. Wortis (to be published).

[16] For the classical XY model $\mathfrak{M}^{zz}(1,2)$ vanishes, if $1\neq2$ and there is no magnetic field in the z direction.

[17] C. Domb and M. F. Sykes, Proc. Roy. Soc. (London) **240A**, 214 (1967).

[18] The nth roots $a_n{}^{1/n}$ for the susceptibility series have been calculated. They show a slight upward curvature (indicating, if it continues, $\gamma<1$) for $n<6$, changing over to a slight downward curvature ($\gamma>1$) for $n>6$.