Japan 18, 1025 (1963).

[7]S. Doniach, Proc. Phys. Soc. (London) 91, 86 (1967).

[8]A. Sakurai, Progr. Theoret. Phys. (Kyoto) 39, 312 (1968).

[9]J. Hubbard and K. P. Jain, J. Phys. C 1, 1650 (1968).

[10]P. Richmond and G. L. Sewell, J. Math. Phys. 9, 349 (1968).

[11]L. G. Caron and G. W. Pratt, Jr., Rev. Mod. Phys. 40, 802 (1968).

[12]R. Kishore and S. K. Joshi, Phys. Rev. 186, 484 (1969).

[13]F. Englert and M. M. Antonoff, Physica 30, 429 (1964).

[14]D. N. Zubarev, Usp. Fiz. Nauk 71, 71 (1960) [Sov. Phys. Usp. 3, 320 (1969)].

[15]In fact, random-phase approximation is justified when all three interactions, intra-atomic interaction I, interatomic Coulomb interaction V_{ij}, and the interatomic exchange interaction J_{ij}, are small as compared to the bandwidth α. It can be shown (Ref. 5) that $I > V_{ij} > J_{ij}$. Therefore, $I \ll \alpha$ implies that V_{ij}, $J_{ij} \ll \alpha$.

[16]D. R. Penn, Phys. Rev. 142, 350 (1966).

[17]M. J. Morris and J. F. Cornwell, J. Phys. C 1, 1145 (1968).

[18]G. A. Baker, Jr., H. E. Gilbert, J. Eve, and G. S. Rushbrooke, Phys. Rev. 164, 800 (1967).

[19]E. C. Stoner, Proc. Roy. Soc. (London) 165, 372 (1938).

[20]D. H. Martin, *Magnetism in Solids* (Iliffe, London, 1967); B. L. Rhodes, S. Legvold, and F. H. Spedding, Phys. Rev. 109, 1547 (1958); D. E. Hegland, S. Legvold, and F. H. Spedding, *ibid.* 131, 158 (1962).

[21]W. Langer, M. Plischke, and D. Mattis, Phys. Rev. Letters 23, 1448 (1969).

[22]S. V. Tyablikov, Ukr. Mat. Zh. 11, 287 (1959).

[23]J. Kanamori, Progr. Theoret. Phys. (Kyoto) 30, 276 (1963).

[24]R. D. Mattuck, Phys. Letters 28A, 407 (1968).

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Universality of Critical Correlations in the Three-Dimensional Ising Ferromagnet*

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Evidence from exact enumeration series is presented to support the hypothesis that the functional form of spin-spin correlations for three-dimensional zero-field Ising ferromagnets in their high-temperature critical region is independent of lattice and spin magnitude.

I. INTRODUCTION

There is strong evidence, both theoretical[1] and experimental,[2] that the critical properties of a system undergoing a thermodynamic phase transition depend crucially on both the spatial dimensionality of the system and the symmetry of the ordering in the ordered phase.[3] In order to develop a first-principles theory of the critical region, it is important to know within these restrictions, i.e., for fixed dimensionality and symmetry, just how universal critical behavior is.[4]

Are critical properties independent of such details as spin magnitude and lattice type, or are they not? Results based on exact perturbation series for magnetic models strongly suggest that the critical exponents are independent of lattice type.[1,5] The evidence that the exponents do not depend on spin magnitude is somewhat weaker but still convincing.[6,7] The logically next and stronger hypothesis is that the functional forms of the equation of state and of the critical correlations are universal. Recent series evidence suggests that the equation of state is lattice independent both above and below T_c.[8] We present below evidence that the critical correlations are universal with respect to lattice type, and we investigate their dependence on spin magnitude.

II. MOMENT-RATIO TEST

It is generally believed that the critical spin-spin correlation function of the three-dimensional Ising model in zero magnetic field has the spherically symmetrical scaling form[9]

$$\Gamma(\vec{r}, T) \equiv \langle S^z_{\vec{r}} S^z_{\vec{0}} \rangle - \langle S^z_{\vec{r}} \rangle \langle S^z_{\vec{0}} \rangle = (a/r)^{1+\eta} D(\kappa r) , \qquad (1)$$

where $r = |\vec{r}|$, the inverse correlation length $\kappa(T) \equiv \xi^{-1}(T) = \kappa_0 \epsilon^\nu$, $\epsilon \equiv 1 - T_c/T$, η and ν are the conventionally defined[1] critical indices, and T_c, κ_0, and a are constants known to depend on both lattice type and spin magnitude. We assume that (1) holds for r large and κ small.[10] This paper examines the universality of the function $D(x = \kappa r)$ for $T \geq T_c$.

Only for the fcc lattice and $S = \frac{1}{2}$ are existing series data good enough to infer D directly.[10] For other situations we probe D by examining the spherical moments $\mu_n \equiv \sum_{\vec{r} \neq 0} r^n \Gamma(\vec{r}, T)$. As $\kappa \to 0$, the correlation length becomes longer than any fixed lattice spacing and one may convert the divergent part of the sum to an integral. Using (1), one finds[11]

$$\mu_n(T) = 4\pi a^{1+\eta} U_n \kappa^{-n-2+\eta} + (\text{less-singular terms}), \qquad (2)$$

provided $n > -2+\eta$, where

$$U_n = \int_0^\infty dx\, x^{n+1-\eta} D(x) \,. \tag{3}$$

Moment ratios such as $\mu_n \mu_m / \mu_k \mu_l$ with $n+m=k+l$ are finite at T_c $(= U_n U_m / U_k U_l)$ and independent of the nonuniversal constants κ_0 and a. For convenience we will analyze the symmetrical quantities

$$R_{nm}(T) \equiv \mu_n \mu_m / (\mu_{(n+m)/2})^2 \,. \tag{4}$$

Universality of the numbers $R_{nm}(T_c) = U_n U_m / (U_{(m+n)/2})^2$ provides direct evidence for the universality of $D(x)$.

It is important to examine which moments test universality most sharply. For sufficiently large n, U_n depends predominantly on $D(x)$ at large $x = \kappa r$. However, it is known[10,12] that for $x \gtrsim \eta$ the correlations are of the Ornstein-Zernicke (OZ) form $D(x)/x^{1+\eta} \sim x^{-1} e^{-x}$. If the maximum of the integrand of (3) is in the OZ region, then $x_{\max} = n+1$ and the corresponding moments and moment ratios probe nothing more than the well-known OZ structure. The crucial values of n and m in (4) are, therefore, $-2+\eta < m,\ n < -1+\eta$. If either n or m violate the lower bound, the estimate (2) fails. If both n and m violate the upper bound, one verifies easily that OZ

$$R_{nm}(T_c) = \Gamma(n+2)\Gamma(m+2)/[\Gamma(\tfrac{1}{2}(n+m)+2)]^2 \,. \tag{5}$$

III. ANALYSIS

We have available the high-temperature series through order $(J/kT)^{12}$ for the correlation function $\Gamma(\vec{r}, T)$ of the three-dimensional Ising model for various lattices and spin magnitudes.[7,13] We form 12th-order series for the spherical moments $\mu_n(T)$ and the moment ratios $R_{nm}(T)$. Extrapolation of these series to T_c provides the needed information, as explained after (4). A basis for this extrapolation is provided by scaling.

According to (2), the leading divergence of μ_n should go as $\kappa^{-n-2+\eta} \sim \epsilon^{-\gamma-n\nu}$ $[\gamma = \nu(2-\eta)]$, an hypothesis which is borne out by careful analysis.[7,13] Thus,

$$\mu_n = 4\pi a^{1+\eta} U_n [\epsilon^{-\gamma-n\nu} + B_n(T)] \,, \tag{6}$$

where $B_n(T)$ is less singular than $\epsilon^{-\gamma-n\nu}$. For $S=\frac{1}{2}$, $B_n(T)$ may be analytic. For $S > \frac{1}{2}$, the evidence[7] suggests that $\epsilon^{\gamma+n\nu} B_n(T)$ may vanish with ϵ like ϵ^σ, $\frac{1}{2} \lesssim \sigma < 1$. The analysis outlined below assumes for simplicity that $B_n(T)$ is nonsingular. Results in practice are independent of any singularity assumed for $B_n(T)$ provided that it is appreciably less singular than the leading term (unless $\gamma + n\nu \approx 0$). It follows from (4) and (6) that $R_{nm}(T)$ may be expanded for small ϵ as

$$R_{nm}(T) = R_{nm}(T_c)[1 + \epsilon^{\gamma+n\nu} B_n(T) + \epsilon^{\gamma+m\nu} B_m(T) - 2\epsilon^{\gamma+(n+m)\nu/2} B_{(n+m)/2}(T) + \cdots] \,. \tag{7}$$

Our extrapolation procedure exploits the most important (i.e., most slowly convergent) of these singularities. Suppose, for example,

$$R_{nm}(T) = \sum_{l=1}^{\infty} \rho_{nm}^{(l)} (J/kT)^l \sim R_{nm}(T_c)(1 + B\epsilon^x) \,. \tag{8}$$

This predicts that the partial sums

$$R_{nm}^N(T) \equiv \sum_{l=1}^{N} \rho_{nm}^{(l)} (J/kT)^l$$

approach $R_{nm}(T)$ for T near T_c in the same way that the partial sums in the Taylor expansion

$$(1 - T_c/T)^x \equiv \sum_{l=0}^{\infty} c_l(x)(T_c/T)^l$$

approach ϵ^x. Thus

$$R_{nm}(T) - R_{nm}^N(T) = B f_N(T) \,,$$

$$f_N(T) = \sum_{l=N+1}^{\infty} c_l(x)(T_c/T)^l \tag{9}$$

which holds for $T \approx T_c$. If we put $T = T_c$, then the unknowns in (9) are $R_{nm}(T_c)$ and B; thus any two consecutive values of N yield a pair of linear equations in two unknowns from which $R_{nm}(T_c)$ may be determined. Successive estimates of $R_{nm}(T_c)$ improve as N increases, since[14] for large N, $f_N(T) \sim 1/N^x$, and corrections to (9) from additional terms[15] on the right-hand side of (8) $(+C\epsilon^y + \cdots)$ vanish as $1/N^y$, $y > x$. To include in the analysis these more convergent terms of (8), one can use three consecutive values of N and solve three linear equations for $R_{nm}(T_c)$, B, C, and so forth. One thus builds up a table of estimates for $R_{n,m}(T_c)$ much like an ordinary Neville table.[16]

IV. DEPENDENCE OF SPIN-$\frac{1}{2}$ CRITICAL CORRELATIONS ON LATTICE STRUCTURE

In extrapolating the spin-$\frac{1}{2}$ ratios we use the well-established values of the critical indices[13] $\gamma = 1.25$ and $\nu = 0.638^{+0.002}_{-0.001}$, and assume that the $B_n(T)$'s are analytic in ϵ. Shown in Table I are the results of such extrapolations for various ratios of interest for the three cubic lattices as well as the OZ predictions for these ratios. Ratios with only large moments agree well with the OZ result. Even though ratios with small moments deviate significantly from OZ, they are independent of lattice effects to within uncertainties.

These results are open to the criticism that, even though the ratios depend most strongly on the large r behavior of $\Gamma(\vec{r}, T)$, our series derive most of their information from correlations at short distances. In an attempt to test the effect of the short-range correlations on these ratios, we formed the ratio series omitting nearest-neighbor correlations, and extrapolated the ratios as described above. We found that the tables were much less

TABLE I. Extrapolated $S=\frac{1}{2}$ moment ratios $R_{nm}(T_c)$ for the cubic lattices with corresponding OZ values.

R_{nm} n	m	OZ	fcc	bcc	sc
$\frac{3}{4}$	$-\frac{7}{4}$	7.425	8.29 ±0.10	8.30 ±0.34	8.1 ±0.3
$\frac{5}{4}$	$-\frac{7}{4}$	10.929	12.25 ±0.20	12.30 ±0.10	12.34 ±0.11
$\frac{7}{4}$	$-\frac{7}{4}$	16.036	17.74 ±0.15	17.75 ±0.10	17.68 ±0.20
$\frac{1}{2}$	$-\frac{3}{2}$	3.000	3.08 ±0.02	3.10 ±0.06	3.11 ±0.07
1	$-\frac{3}{2}$	4.197	4.33 ±0.07	4.33 ±0.06	4.37 ±0.06
$\frac{3}{2}$	$-\frac{3}{2}$	5.891	6.07 ±0.06	6.076 ±0.030	6.07 ±0.07
$\frac{1}{4}$	$-\frac{5}{4}$	1.7677	1.790 ±0.010	1.80 ±0.03	1.796 ±0.025
$-\frac{1}{4}$	$-\frac{5}{4}$	1.3709	1.385 ±0.010	1.386 ±0.035	1.386 ±0.060
$-\frac{1}{2}$	−1	1.0787	1.0810 ± 0.0010	1.0825 ± 0.0034	1.082 ±0.007
$\frac{1}{2}$	−1	1.5718	1.580 ±0.010	1.587 ±0.010	1.588 ±0.011
2	1	1.08657	1.0865 ± 0.0003	1.0865 ± 0.0003	1.0864 ± 0.0003

well behaved than previously and that there were large, slow variations in the table about the values quoted in Table I. That is, from these extrapolations we quote approximately the same values as in Table I with larger uncertainties.

We feel that this evidence rather strongly supports the hypothesis that the critical correlations are universal with respect to lattice type.

V. DEPENDENCE OF fcc CRITICAL CORRELATIONS ON SPIN MAGNITUDE

Susceptibility and moment series for $S>\frac{1}{2}$ are harder to analyze than those for $S=\frac{1}{2}$. Careful analysis[7] of long series has only been done for the fcc lattice. The presence of confluent singularities of the form $\chi\sim A\epsilon^{-\gamma}(1+B\epsilon^{x})$, where $x\sim\frac{1}{2}$ (A and B are spin dependent), has been suggested. It can plausibly be argued that $\gamma=\frac{5}{4}$ for all S; however, the correlation index is ambiguous and the $S>\frac{1}{2}$ data can be interpreted either with the scaling value $\nu=0.625=(2-\alpha)/d$ or with the $S=\frac{1}{2}$ value $\nu=0.638$. The scaling choice $\nu=0.625$ [which implies via $\gamma=\nu(2-\eta)$ that $\eta=0$] is, of course, already a violation of universality. Recent work by Migdal[17] suggests a mechanism by which such apparent violations may be produced in three-dimensional systems.

Our extrapolative estimates of $R_{nm}(T_c)$ are very sensitive to the values of γ and ν assumed. This is particularly true of ratios containing small moments like $\mu_{-7/4}$ for which $\gamma+n\nu\sim 0$. To illustrate the situation, we have analyzed the moment ratios $R_{n,-7/4}(T_c)$ with $n=\frac{3}{4}$ and $\frac{5}{4}$ for $S=\frac{1}{2}$, 1, 2, ∞. In this analysis we take

$$R_{n,-7/4}(T)=R_{n,-7/4}(T_c)+B\epsilon^{\gamma-7\nu/4} + (\text{higher-order terms}). \quad (10)$$

The ϵ dependence of the higher-order corrections is conjectural as mentioned above, and thus, in order not to prejudice the analysis, we incorporate the higher-order corrections by an ordinary Neville table. These tables are somewhat less regular than those used in Sec. IV and uncertainties are corre-

TABLE II. Selected moment ratios for $S=\frac{1}{2}$, 1, 2, ∞ for different assumed values of the correlation index ν. $\gamma=\frac{5}{4}$ was assumed throughout.

	ν \ S	$\frac{1}{2}$	1	2	∞
$R_{3/4,-7/4}(T_c)$					
	0.625	7.50 ± 0.15	7.60 ± 0.15	7.70 ± 0.25	7.5 ±0.2
	0.638	8.2 ±0.1	8.28 ± 0.15	8.33 ± 0.15	8.2 ±0.2
$R_{5/4,-7/4}(T_c)$					
	0.625	11.1 ±0.2	11.20 ± 0.15	11.20 ± 0.15	11.00 ± 0.15
	0.638	12.20 ± 0.10	12.10 ± 0.20	12.20 ± 0.20	12.20 ± 0.15

spondingly larger. The analysis was done with $\nu = 0.638$ and $\nu = 0.625$. Results are shown in Table II. OZ values for the two moments shown are 7.425 and 10.929.

If $\nu = 0.638$, then these results are consistent with universality. If $\nu = 0.625$ ($\eta = 0$), then our extrapolations are in suggestive agreement with OZ. The close connection between ν and the moment-ratio extrapolants precludes resolution of this ambiguity.

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[1]M. E. Fisher, Rept. Progr. Phys. 30, 615 (1967); L. P. Kadanoff *et al.*, Rev. Mod. Phys. 39, 395 (1967).

[2]P. Heller, Rept. Progr. Phys. 30, 731 (1967).

[3]David Jasnow and Michael Wortis, Phys. Rev. 176, 739 (1968); R. B. Griffiths, Phys. Rev. Letters 24, 1479 (1970).

[4]For example, if universality fails, then it is unlikely that there exists a unique critical operator algebra for each dimensionality and symmetry. See L. P. Kadanoff, Phys. Rev. Letters 23, 1430 (1969).

[5]C. Domb, Advan. Phys. 9, 149 (1960); C. Domb and M. F. Sykes, Proc. Roy. Soc. (London) A240, 214 (1957).

[6]Spin dependence of the Ising and Heisenberg models was first studied by C. Domb and M. F. Sykes, Phys. Rev. 128, 168 (1962). Heisenberg-model work was also done by ($S=\frac{1}{2}$) G. A. Baker *et al.*, *ibid.* 164, 800 (1967), and ($S=\infty$) H. E. Stanley, *ibid.* 158, 537 (1967), and has been recently reanalyzed by R. G. Bowers and M. E. Woolf, *ibid.* 177, 917 (1969).

[7]More recent work on the spin-S Ising model using 12-term high-temperature series suggests the presence of confluent singularities in the susceptibility and other moments: D. M. Saul, David Jasnow, and Michael Wortis (unpublished). The apparent spin dependence of γ found in an earlier publication (Jasnow and Wortis, Ref. 3) can be explained in this way while maintaining $\gamma = 1.25$ for all S. The status of ν is less clear. Present data admit a range of values $0.62 < \nu < 0.64$ for $S > \frac{1}{2}$.

[8]P. G. Watson, J. Phys. C 2, 1883 (1969); D. S. Gaunt and C. Domb, *ibid.* 3, 1442 (1970).

[9]L. P. Kadanoff, Physics 2, 263 (1966); M. E. Fisher and R. J. Burford, Phys. Rev. 156, 583 (1967).

[10]M. Ferer, M. A. Moore, and Michael Wortis, Phys. Rev. Letters 22, 1382 (1969). There is evidence that (1) fails in the strong scaling limit $\kappa r \to 0$; however, the divergent moments of $\Gamma(\vec{r}, T)$ do not probe this region. Our discussion is therefore limited to the "weak scaling" universality of $D(x)$. See also G. Stell, *ibid.* 24, 1343 (1970).

[11]It is expected, for example, that nearby sites contribute energy-density-like terms $(1 + C\epsilon^{1-\alpha} + \cdots)$. For spins other than $S=\frac{1}{2}$ there appear to be further divergent terms, more singular than $\kappa^{-n-2+\eta}$.

[12]A proof that the correlations have OZ form $T > T_c$, $r \to \infty$ is given by W. J. Camp, thesis (Cornell University, 1970) (unpublished), and M. E. Fisher and W. J. Camp, Phys. Rev. Letters 26, 73 (1971).

[13]M. A. Moore, David Jasnow, and Michael Wortis, Phys. Rev. Letters 22, 940 (1969).

[14]M. F. Sykes, J. L. Martin, and D. L. Hunter, Proc. Phys. Soc. (London) 91, 671 (1967).

[15]Note that convergence is best when $y \gg x$. For this reason we have avoided ratios (4) with weakly singular demoninators.

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

[17]A. A. Migdal, Zh. Eksperim. i Teor. Fiz. 59, 1015 (1970) [Sov. Phys. JETP (to be published)].

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Effect of Band Structure on Spin Fluctuations in Nearly Antiferromagnetic Metals

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A model band structure due to Rice which exhibits a "cusp" Kohn singularity has been used to evaluate the dynamic susceptibility of nearly itinerant antiferromagnets. The spin-fluctuation dispersion relation is derived for such systems, and it is shown that the contribution of the spin fluctuations to the electronic specific heat contains anomalous terms in contrast with the calculations of Moriya.

I. INTRODUCTION

The behavior of spin fluctuations in nearly ferromagnetic metals and alloys has been the subject of many recent research papers.[1] However, spin fluctuations in nearly antiferromagnetic metals and alloys have received little attention. There are two reasons for this situation: (i) The only itinerant antiferromagnets that have been thoroughly investigated experimentally are pure Cr and its alloys. (ii) The band structure of Cr is essential for an understanding of the nature of the antiferromagnetic