SPIN-SPIN CORRELATION FUNCTION OF THE THREE-DIMENSIONAL ISING FERROMAGNET ABOVE THE CURIE TEMPERATURE*

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(Received 20 March 1969)

High-temperature series expansions for the Ising model's spin-spin correlation function are found to order $(J/kT)^{12}$ on the simple cubic, bcc, and fcc latices. Analysis of moment series indicates that the scaling form of the correlation function is correct, at least in the limit κr fixed, $\kappa \to 0$. Values are obtained for the correlation indices ν and η—the latter by two methods, thereby providing a direct check on the scaling law.

The use of exact series expansions in the study of critical phenomena has produced much information on the critical indices describing continuous phase transitions.[1-3] Reported here are some results found by a new method of obtaining such series expansions, a method which only requires a modest amount of computer programming and which can be applied to any of the spin Hamiltonians usually studied.[3] To illustrate the potential of the method, it has been used to find the high-temperature series expansion of the spin-spin correlation function of the Ising ferromagnet on the three-dimensional lattices with cubic symmetry through order $(J/kT)^{12}$. The basis of the method is not new, but it is the first time to our knowledge that it has actually been used for obtaining series expansions. It is based on the linked-cluster expansion developed for the Ising model by Englert[4] but completely renormalized in analogy with the work of De Dominicis for the classical gas.[5] The vertex-renormalized version of the Englert expansion has been used elsewhere in deriving high-temperature expansions for the anisotropic classical Heisenberg model on various lattices.[6] The completely renormalized version of the Englert expansion[7] has the effect of expressing the interaction potential between individual spins in terms of a diagrammatic expansion in certain quantities closely related to the spin-spin correlation function $\Gamma(\vec{r}, T)$. At temperatures greater than the critical temperature this equation may be iterated as a nonlinear integ. al equation, giving $\Gamma(\vec{r}, T)$ as a power series in J/kT, where J is the interaction energy between parallel spins. Numerical iteration of the integral equation to twelfth order in J/kT took 20 min for the fcc lattice on an IBM 360/75 computer, but only 2 min for the simple cubic lattice. 42 diagrams are needed to twelfth order for the fcc lattice. The lattice summations involved in evaluating the diagrams are unrestricted rather than being of the "excluded-volume" type.[8] It is this feature which is ultimately responsible for the great saving in computing time.

The spin-spin correlation function of the Ising model is of great interest. The range $\xi(T, H)$ of correlations becomes infinite at the critical point and is expected to behave for $T \gtrsim T_c$ in zero field as[9]

$$\xi^{-1}(T, 0) \equiv \kappa(T) = \kappa_0[1-(v/v_c)]^{\nu}, \tag{1}$$

where we use the conventional variable[1] $v = \tanh(J/kT)$. Scaling[3,10,11] predicts that the correlation index ν is related to the high-temperature specific heat index α by

$$d\nu = 2-\alpha, \tag{2}$$

where d is the dimensionality of the system. Equation (2) holds for the Ising model in two dimensions. In three dimensions, insertion of the widely accepted value[12] $\alpha = \frac{1}{8}$ into (2) yields $\nu = 0.625$, which disagrees with the result $\nu = 0.643 \pm 0.0025$ found by Fisher and Burford[9] on the basis of rather short series. Only for the Ising model are the critical indices known to sufficient accuracy to permit a meaningful check of (2), so this discrepancy is probably the only real evidence for the failure of the scaling laws. It therefore becomes important to ascertain whether the discrepancy is merely a consequence of using too-short series.

Kadanoff[10,11] has suggested that near T_c in zero field the correlations scale according to

$$\Gamma(\vec{r}, T) = D(\kappa r)/r^{d-2+\eta}, \tag{3}$$

provided that $r \gg a$ (the nearest-neighbor lattice spacing) and $a\kappa = a\kappa(T) \ll 1$ but for arbitrary values of the product κr. This provocative form is known[13] to hold for the Ising model in two dimensions, and it is important to discover whether it remains valid in three dimensions. The probable failure of the scaling relation (2) suggests that there may be a breakdown in the scaling form of the correlation function, and this is indeed what we have found. However, the breakdown is such that Eq. (3) still holds, but now for the limit κr fixed, $\kappa a \to 0$, i.e., scaling holds provided that distances are measured in units of the coherence length. The analysis in the rest of this Letter is some of the evidence that this weaker form of scaling holds. We hope to report full details on the breakdown of the stronger form of the scaling hypothesis in a future communication.

In order to extract the correlation index ν from the correlation function and to test the scaling relation (3), we form the spherical moment series,[9]

$$\mu_t = \sum_{\vec{r}} (r/a)^t \Gamma(\vec{r}, T) = \sum_n m_n^{(t)} v^n. \tag{4}$$

The quantities $m_n^{(0)}$ are the coefficients of the usual dimensionless susceptibility series; $m_n^{(2)}$ are the coefficients of the second moment series. Table I contains susceptibility and second moment coefficients for the three cubic lattices. Quite generally, we may expect that μ_t has a leading exponential singularity at the critical point, which we may write

$$\mu_t \sim [1-(v/v_c)]^{-(\gamma + t\nu_t)}, \text{ as } v \to v_c, \tag{5}$$

where γ is the susceptibility index ($t=0$). Substitution of (3) into (4) and comparison with (5) yields the scaling relations

$$\gamma = (2-\eta)\nu \tag{6}$$

and $\nu_t = \nu$. Hence, a necessary test of the scaling of correlations (3) is the equality of the ν_t determined from the moment series for different values of t. This test can only provide evidence for scaling in the limit of κr fixed, $\kappa a \to 0$.

Using the conventional ratio methods of analysis[14] on various moment series we estimate that $v_c(\text{fcc}) = 1/9.828$, $v_c(\text{bcc}) = 1/6.4045$, and $v_c(\text{sc}) = 1/4.584$, with an uncertainty of probably no more than 1 part in 10^4. We find the expected result for γ of 1.250 with an uncertainty in the extrapolation of no more than ± 0.002. There seems no reason to doubt that γ is exactly 5/4.[1] The moment series with values of t ranging from -2 to 10 were then extensively analyzed by a variety of methods. Outside this range all methods of analysis tend to break down as a result of the series becoming very irregular (for large negative t) or of great curvature in plots of $\nu_{t,n}$ vs $1/n$ [see Eq. (8)] for large positive t). One method used to find ν_t was first to divide the μ_t series by the susceptibility series to obtain a new series which should behave, as $v \to v_c$, like $(1-v/v_c)^{-t\nu_t}$. Denoting the ratio of successive terms in this new series by ρ_n, a sequence of estimates for ν_t is given by

$$\nu_{t,n} = n(v_c \rho_n - 1)/t + 1/t. \tag{8}$$

A plot of $\nu_{t,n}$ vs $1/n$ is usually linear, provided $t > 0$. Define the (linearly) extrapolated intercepts by

$$\nu_{t,n}' = n\nu_{t,n} - (n-1)\nu_{t,n-1} \tag{9}$$

Table I. Coefficients for the expansion of the zeroth and second correlation moments in powers of v for the spin-$\frac{1}{2}$ Ising ferromagnet.

	sc		bcc		fcc	
n	$m_n^{(0)}$	$m_n^{(2)}$	$m_n^{(0)}$	$m_n^{(2)}$	$m_n^{(0)}$	$m_n^{(2)}$
1	6	6	8	8	12	12
2	30	72	56	128	132	288
3	150	582	392	1416	1404	4908
4	726	4032	2648	13 568	14 652	72 096
5	3510	25 542	17 864	119 240	151 116	973 116
6	16 710	153 000	118 760	992 768	1 546 332	12 432 096
7	79 494	880 422	789 032	7 948 840	15 734 460	152 805 372
8	375 174	4 920 576	5 201 048	61 865 216	159 425 580	1 825 058 688
9	1 769 686	26 879 670	34 268 104	470 875 848	1 609 987 708	21 320 627 196
10	8 306 862	144 230 088	224 679 864	3 521 954 816	16 215 457 188	244 722 705 888
11	38 975 286	762 587 910	1 472 595 144	25 965 652 936	162 961 837 500	2 768 965 884 780
12	182 265 822	3 983 525 952	9 619 740 648	189 180 221 184	1 634 741 163 188[a]	30 958 965 878 880[a]

[a]Comparison with some unpublished work of Dr. M. F. Sykes indicates that these two numbers may be in error. The magnitude of the possible error is such that it could have no effect on the results here presented.

for the fcc lattice, and by

$$\nu_{t,n}' = \tfrac{1}{2} n \nu_{t,n} - \tfrac{1}{2}(n-2)\nu_{t,n-2} \quad (10)$$

for the sc and bcc lattices. For $n = 7$ to $n = 12$, we find

$$\nu_{2,n}' = 0.6362,\ 0.6365,\ 0.6369,\ 0.6374,\ 0.6377,\ 0.6378 \quad (11)$$

for the fcc lattice and

$$\nu_{2,n}' = 0.6410,\ 0.6387,\ 0.6375,\ 0.6386,\ 0.6381,\ 0.6385 \quad (12)$$

for the sc lattice. For values of t which are positive, this and other ratio methods of analysis give very similar results for ν_t, all around 0.638. For negative values of t the same methods yield values of ν_t that decrease with t, falling below 0.625 for $t < -2$. As $t \to -\infty$, one would expect the resulting series to behave like the internal energy, for then any finite series will look very similar to the spin-spin correlation function to a site close to the origin. Hence the apparent decrease in ν_t is not very surprising.

There is, however, another method of analysis which yields constant values for ν_t throughout the entire range $-2 < t < 10$ and for the superiority of which an a priori argument can be made. This method starts by forming the coefficients $\langle R_n^{tt'}\rangle$ defined by

$$m_n^{(t)} = \langle R_n^{tt'}\rangle m_n^{(t')}. \quad (13)$$

If the scaling form (3) holds, the coefficients $\langle R_n^{tt'}\rangle$ should be proportional to $n^{(t-t')\nu}$ for large n, so that the ratio of successive coefficients $\langle R_n^{tt'}\rangle$ should approach unity with a slope proportional to $(t-t')\nu$, when plotted as a function of $1/n$. One can therefore determine ν without first having to estimate the critical temperature. This procedure by itself is quite successful, but the most consistent results are obtained by analyzing the logarithmic derivative with respect to $\ln x$ of the generating function

$$G(x, t, t') = \sum_n \langle R_n^{tt'}\rangle x^n \quad (14)$$

for $t > t'$.[15] Each term in the resulting series would be an estimate of $1 + (t-t')\nu$ if the scaling form (3) were valid. It can be shown that working with the ln derivative series considerably reduces the amplitude of certain types of competing singularities. This seems to happen here, as values of ν always around 0.638 are recovered if t and t' are kept within the range from -2 to 10. As an example, for $t = 2$ and $t' = 0$, on the fcc lattice, the following sequence of estimates for ν_2 is obtained on going from the fifth to the twelfth term; 0.638 69, 0.638 87, 0.638 10, 0.638 21, 0.638 43, 0.638 49, 0.638 41, and 0.638 38. We shall conclude therefore that

$$\nu_t = \nu = 0.638^{+0.002}_{-0.001} \quad (15)$$

and that the scaling form (3) is valid within the accuracy of our extrapolations. It should be therefore permissible to use the scaling relation (6) to find η, which is then $0.041^{+0.006}_{-0.003}$.

Alternatively, the index η can be determined directly by analyzing the decay of correlations at the critical point,

$$\Gamma_c(\vec{r}) \equiv \Gamma(\vec{r}, T \equiv T_c) = D(0)/r^{d-2+\eta}, \quad (16)$$

provided only that $r \gg a$. For each lattice separation $\vec{r}$, $\Gamma_c(\vec{r})$ can be estimated from the series expansion by extrapolating[16] the nth partial sum versus $(n-\delta)^{-7/8}$. In Fig. 1 we have plotted $\ln[(r/a)\Gamma_c(\vec{r})]$ vs $\ln(r/a)$ on the fcc lattice for those values of r for which reasonably consistent extrapolation seems possible with the number of terms available. The slope of this plot gives $-\eta$. The precision of this approach is limited, but the value of η obtained is entirely compatible with the results quoted above, thus providing a direct check of the scaling law (6). We remark[9] that on the plane square lattice the asymptotic expression (16) is accurate to within 1.5% even for

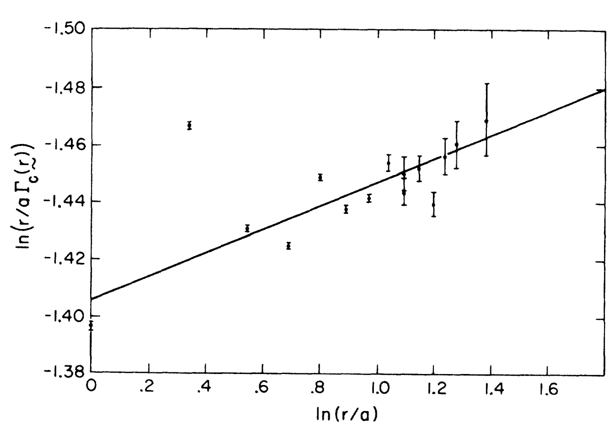

FIG. 1. A plot of $\ln[(r/a)\Gamma_c(\vec{r})]$ vs $\ln(r/a)$. The straight line corresponds to an η of 0.041. The error bars are an attempt at representing the uncertainties in the extrapolations.

sites near the origin. It is therefore not unreasonable to hope that the nearest and next-nearest-neighbor correlations bracket the extrapolation to small r of the asymptotic form (16).

We should like to thank Dr. M. F. Sykes for allowing us to compare our results for the susceptibility and energy density with some of his unpublished work, thereby providing an important check on the calculations. We are indebted to Professor L. P. Kadanoff for many interesting discussions.

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*Work supported in part by the National Science Foundation under Grant No. NSF GP-7765 and the Advanced Research Projects Agency under Contract No. ARPA SD-131.

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[1]C. Domb and M. F. Sykes, Proc. Roy. Soc. (London), Ser. A 240, 214 (1957).

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

[3]M. E. Fisher, Rept. Progr. Phys. 30, 615 (1967), gives an extensive list of further references.

[4]F. Englert, Phys. Rev. 129, 567 (1963). See also C. Bloch and J. S. Langer, J. Math. Phys. 6, 554 (1965).

[5]C. De Dominicis, J. Math. Phys. 3, 983 (1962).

[6]D. Jasnow and M. Wortis, Phys. Rev. 176, 739 (1968); D. Jasnow and M. A. Moore, Phys. Rev. 176, 751 (1968).

[7]M. Wortis, D. Jasnow, and M. A. Moore, to be published.

[8]For a review of the conventional method of obtaining series expansions see C. Domb, Advan. Phys. 9, 149 (1960).

[9]M. E. Fisher and R. J. Burford, Phys. Rev. 156, 583 (1967).

[10]L. P. Kadanoff, Physics (N.Y.) 2, 263 (1966).

[11]L. P. Kadanoff et al., Rev. Mod. Phys. 39, 395 (1967).

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

[13]L. P. Kadanoff, Nuovo Cimento 44B, 276 (1966).

[14]C. Domb and M. F. Sykes, J. Math. Phys. 2, 63 (1961).

[15]A similar approach has been used by D. S. Gaunt, Proc. Phys. Soc. (London) 92, 150 (1967).

[16]See Fisher and Burford, Ref. 9, p. 611.

NUCLEAR HYPERFINE CONTRIBUTION TO THERMAL CONDUCTIVITY OF HOLMIUM

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(Received 17 February 1969)

Thermal conductivity of a holmium single crystal has been measured in the temperature range 0.6 to 4.2°K. Around 1°K there is a total enhancement of over 30 % in the conductivity value and the Lorenz number increases sharply to beyond 3.8×10^{-8} W Ω/deg^2. When correlated with specific heat data, this extra contribution appears to be a nuclear hyperfine effect. A possible mechanism is proposed.

This is to report the first observation of what we believe is a nuclear hyperfine contribution to the thermal conductivity of holmium around 1°K. A unique feature in rare-earth ferromagnets has been the large values obtained for the calculated Lorenz number, the ratio of thermal to electrical conductivity. Around 4°K, this value ranges from (5 to 10)$\times10^{-8}$ W Ω/deg^2 as compared with the standard Sommerfeld value of 2.45×10^{-8} W Ω/deg^2 expected in ordinary metals.[1] To account for this, the presence of additional heat carriers like magnons and/or phonons have been suggested.[2-4] In rare-earth ferromagnets, in addition to electrons, phonons and spin disorder, there is a possibility of a new mechanism of heat transport arising from the nuclear hyperfine field. This nuclear contribution (arising from the interaction of the nuclei with the hyperfine field and the Rudermann-Kittel-type indirect exchange interaction coupling the nuclear spins and the $4f$ electrons with the conduction electrons), as in specific heat[5] and thermal expansion,[6,7] would ordinarily be significant only at very low temperatures ($T < 0.5$°K). In terbium and holmium, however, this can be large even at higher temperatures. Our experimental data indicate that in holmium this contribution is significant below about 1.2°K, enhancing the total thermal conductivity by as much as 30% or more.

Our thermal-conductivity measurements on a single-crystal holmium specimen in the temperature range 0.6 to 4.2°K are presented in Fig. 1. The electrical resistivity, measured by the standard four-probe technique, was found to have a