PHYSICAL REVIEW B VOLUME 4, NUMBER 11 1 DECEMBER 1971

Spin-Spin Correlations of the Classical Heisenberg Ferromagnet on the fcc Lattice, for Temperatures above T_C †

M. Ferer*

Department of Physics, University of Illinois at Urbana–Champaign, Urbana, Illinois 61801

(Received 2 April 1971)

High-temperature series are presented for the spin-spin correlation function of the spin-infinity nearest-neighbor Heisenberg ferromagnet on the fcc lattice. Our zero-field series are to tenth order in the interaction, while our finite field series are to eighth order in the interaction. Previous analysis of these series indicated $\gamma = 1.405 \pm 0.020$ and $\nu = 0.717 \pm 0.007$. These series are used to determine the true correlation length. Further examination of these series indicates that, where the inverse correlation length κ is not much smaller than the momentum transfer k (explicitly $\kappa^2/k^2 > 0.08$), the correlations in momentum space are well represented by the Ornstein-Zernike form $\mu^\eta(k^2+\mu^2)$, where η has been found to be 0.040 ± 0.008, not zero as in mean-field theories.

I. INTRODUCTION

In the preceding paper, hereafter referred to as I, we analyzed series derived from the correlation-function series in order to determine the form of the leading critical singularities of some of the physical properties.[1] There is also interest in the functional dependence of the critical correlations on reduced temperature $\epsilon \equiv 1 - T_C/T$ and spin separation $\vec{r}$. This dependence has been investigated for the spin-$\frac{1}{2}$ Ising model in which only the z components of the spins are coupled[2-4]; but, to our knowledge, this is the first such investigation for the Heisenberg model which has isotropic spin-spin coupling.

The classical (spin-infinity) Heisenberg model is a system of classical unit vectors $\vec{S}(\vec{r}_i)$ at all sites i of the lattice interacting with their nearest neighbors and with an external field H applied in the z direction through the Hamiltonian

$$-\beta\mathcal{H} = v \sum_{\langle i,j\rangle} \vec{S}(\vec{r}_i)\cdot\vec{S}(\vec{r}_j) + h\sum_i S^z(\vec{r}_i),$$

$$v = \beta J, \qquad h = \beta m H \qquad (1.1)$$

where the first sum is over all nearest-neighbor pairs, the second is over all lattice sites, J is the coupling strength, and $\beta = 1/kT$. We consider the correlations between $S^\alpha(\vec{0})$ and $S^\beta(\vec{r})$, that is,

$$\Gamma^{\alpha\beta}(\vec{r}, T, h) = \langle S^\alpha(\vec{0}) S^\beta(\vec{r})\rangle - \langle S^\alpha(\vec{0})\rangle\langle S^\beta(\vec{r})\rangle \ , \qquad (1.2)$$

where $\langle X\rangle$ denotes the thermal average of X, that is $\langle X\rangle = \mathrm{Tr}(Xe^{-\beta\mathcal{H}})/\mathrm{Tr}e^{-\beta\mathcal{H}}$. In zero field, one finds $\Gamma^{\alpha\beta}(\vec{r}, T, h=0) = \Gamma^{zz}(\vec{r}, T, h=0)\delta_{\alpha\beta}$, $\alpha\beta = x,\ y,$ or z; thus, we drop the superscript labels and consider only the correlations between the z components of spin. A rearrangement of these series, which will be discussed in Sec. III, is presented in Table I so that the reader might check the assertions in either of these papers.

It has been postulated that $\Gamma(\vec{r}, T, h=0)$ has the scaling form $D(\kappa r)/r^{d-2+\eta}$ for $\kappa a \ll 1$ and for $r/a \gg 1$, where $r = |\vec{r}|$, $\kappa = \kappa_0\epsilon^\nu$, d is the dimensionality, and a is the nearest-neighbor distance.[5,6] This assertion has been tested and the form of $D(x)$ determined for the spin-$\frac{1}{2}$ Ising model in both two[2] and three[3,4] dimensions. We use methods identical to those of Ref. 4 to investigate these matters for the Heisenberg model. The scaling form of the spatial correlations implies that, for the correlations in momentum space, one has

$$\Gamma(\vec{k}, T, h) = \sum_{\vec{r}} e^{i\vec{k}\cdot\vec{r}}\,\Gamma(\vec{r}, T, h),$$

$$\Gamma(\vec{k}, T, h=0) = \frac{1}{\kappa^{2-\eta}} f\left(\frac{\kappa}{|\vec{k}|}\right) . \qquad (1.3)$$

Fisher and Burford have parametrized the function $f(x)$ and have determined the parameters for the three-dimensional spin-$\frac{1}{2}$ Ising model on the simple cubic lattice.[3] We use their parametrization for the Heisenberg model and observe that it is qualitatively consistent with our investigations of the spatial correlations. One of the parameters has an importance quite independent of the parametrization. This is the true correlation length κ, which is the solution of the equation $\Gamma^{-1}(i\kappa, T, h) = 0$ and which provides a definition of the inverse correlation length independent of any scaling assumptions. These investigations of the correlations, in both coordinate and momentum space, strengthen the belief that the Ornstein-Zernike form $\kappa^\eta e^{-\kappa r}/r$ [or $\kappa^\eta/(\kappa^2+k^2)$] will be an accurate approximant as long as κr [or κ^2/k^2] is not small.

II. EXTRAPOLATION OF $\Gamma(\vec{r}, T, h=0)$

In this section, we test the scaling prediction

TABLE I. Shown are the coefficients $\mathcal{K}(l, m, n, i, j)$ of the series, Eq. (3.4), for $\frac{1}{3}\Gamma^{-1}(\vec{k}, T, h)$. Because of cubic symmetry, all permutations of l, m, and n are equivalent. In the higher orders, the thirteenth, fourteenth, and fifteenth places after the decimal point may be incorrect because of computer roundoff.

$l\ m\ n$				
		$\mathcal{K}(l, m, n, i, j=0)$		
000	+1.0	+0.0	+1.333 333 333 333 33v^2	+1.777 777 777 777 77v^3
	+3.229 629 629 629 63v^4	+6.637 037 037 037 04v^4	+14.710 593 768 371 6v^6	+34.530 803 057 025 0v^7
	+84.445 500 032 666 6v^8	+212.510 043 882 045v^9	+546.242 819 576 081v^{10}	
110	−0.333 333 333 333 333v	0.0	−0.014 814 814 814 815v^3	−0.059 259 259 259 259v^4
	−0.171 992 945 326 271v^5	−0.459 651 185 576 842v^6	−1.170 333 790 580 70v^7	−2.907 044 757 337 92v^8
	−7.152 559 351 218 25v^9	−17.529 911 529 860 4v^{10}		
200	−0.018 436 213 991 769v^6	−0.092 122 542 295 382v^7	−0.308 502 101 163 216v^8	−0.877 842 117 570 499v^9
	−2.272 386 764 494 61v^{10}			
211	−0.000 877 914 951 989v^6	−0.010 886 145 404 664v^7	−0.062 514 512 175 004v^8	−0.271 800 796 913 326v^9
	−1.016 947 324 044 70v^{10}			
220	−0.000 585 276 634 659v^7	−0.007 364 730 986 130v^8	−0.049 238 115 560 416v^9	−0.240 215 290 344 824v^{10}
222	−0.000 829 141 899 101v^9	−0.009 091 297 058 375v^{10}		
310	−0.003 126 352 690 139v^9	−0.031 429 326 660 909v^{10}		
321	−0.000 022 760 758 014v^9	−0.000 936 225 880 201v^{10}		
330	−0.000 013 006 147 436v^{10}			
		$\mathcal{K}(l, m, n, i, j=2)$		
000	+0.2	+1.6v	+8.871 111 111 111 11v^2	
	+42.287 407 407 407 4v^3	+185.542 603 174 603v^4	+771.289 998 824 219v^5	
	+3085.020 582 402 48v^6	+11986.996 023 209 5v^7	+45535.066 568 770 2v^8	
110	−0.032 592 592 592 593v^2	−0.329 876 543 209 880v^3	−2.104 644 326 866 59v^4	
	−10.914 426 807 761 0v^5	−50.232 494 245 234 2v^6	−214.215 972 264 274v^7	
	−867.741 941 543 211 v^8			
200	−0.043 456 790 123 446v^4	−0.424 559 670 781 902v^5	−2.563 780 887 056 41v^6	
	−12.446 740 401 047 1v^7	−53.560 472 697 515 3v^8		
211	−0.008 296 296 296 319v^4	−0.113 075 445 816 017v^5	−0.892 704 474 494 843v^6	
	−5.365 747 625 549 55v^7	−27.286 441 249 042 5v^8		
220	−0.000 526 748 971 194v^4	−0.016 329 218 107 009v^5	−0.171 993 572 409 044v^6	
	−1.217 911 624 969 53v^7	−6.881 899 799 844 87v^8		
222	−0.008 155 829 904 010v^6	−0.117 699 131 226 556v^7	−1.013 758 829 499 11v^8	
310	−0.015 890 260 632 671v^6	−0.197 565 980 793 730v^7	−1.434 578 498 690 34v^8	
321	−0.001 144 215 820 765v^6	−0.026 505 227 863 630v^7	−0.293 155 302 557 428v^8	
330	−0.000 035 116 598 023v^6	−0.001 923 609 204 134v^7	−0.029 096 628 399 596v^8	

TABLE I (*Continued*).

lmn	$\mathcal{K}(l, m, n, i, j=2)$
332	$-0.002\,718\,740\,034\,979v^8$
400	$-0.013\,276\,024\,957\,343v^8$
411	$-0.011\,186\,587\,401\,130v^8$
420	$-0.003\,827\,709\,203\,861v^8$
422	$-0.000\,407\,157\,439\,011v^8$
431	$-0.000\,148\,205\,050\,923v^8$
440	$-0.000\,002\,341\,106\,807v^8$

$\Gamma(\vec{r}, T, h=0) = D(\kappa r)/r^{1+\eta}$ and determine the form of $D(x)$, using the methods of Ref. 4 to extrapolate our correlation-function series for given values of $\vec{r}$ and T. It is reasonable to expect that the leading singularity of $\Gamma(\vec{r}, T, 0)$ is the energy-density singularity $\epsilon^{1-\alpha}$,[3,4] so that

$$\Gamma(\vec{r}, T, 0) = \Gamma(\vec{r}, T_C, 0) + E(\vec{r})\epsilon^{1-\alpha} + \text{higher orders in } \epsilon \ . \qquad (2.1)$$

This means that the partial sums

$$\Gamma^N(\vec{r}, T, 0) = \sum_{n=0}^{N} Q(\vec{r}, n, j=0)\, v^n$$

approach $\Gamma(\vec{r}, T, 0) = \Gamma^\infty(\vec{r}, T, 0)$ in the same way that the partial sums of the Taylor expansion of

$$\epsilon^{1-\alpha} = \sum_{n=0}^{\infty} C_n(1-\alpha)\left(\frac{v}{v_C}\right)^n$$

approach $\epsilon^{1-\alpha}$, $\epsilon = 1 - v/v_C = 1 - T_C/T$, where $C_n(1-\alpha)$ is the nth Taylor coefficient. Thus, to leading order in $1/N$,

$$\Gamma(\vec{r}, T, 0) - \Gamma^N(\vec{r}, T, 0) = B g_N(1-\alpha, T)\ ,$$
$$g_N(1-\alpha, T) = \sum_{n=N+1}^{\infty} C_n(1-\alpha)\left(\frac{T_C}{T}\right)^n\ , \qquad (2.2)$$

where, using the values of T_C and α from I, the only unknowns are $\Gamma(\vec{r}, T, 0)$ and B. The large uncertainty in α, almost 50%, might be thought to greatly reduce the accuracy of the extrapolation; but actually the uncertainty in $1-\alpha$ is less than 6% and will not greatly affect the accuracy of the extrapolations. Equation (2.2) for two consecutive values of N yields a pair of linear equations in two unknowns, $\Gamma(\vec{r}, T, 0)$ and B, giving an estimate for $\Gamma(\vec{r}, T, 0)$. We approximate the higher orders in ϵ of Eq. (2.1) by the assumption

$$\Gamma(\vec{r}, T, 0) - \Gamma^N(\vec{r}, T, 0) = g_N(1-\alpha, T)(B_0 + B_1/N + B_2/N_2 + \cdots)\ . \qquad (2.3)$$

We can then use three consecutive N values in Eq. (2.3) with $B_i = 0$, $i > 1$, and solve the three linear equations for another estimate of $\Gamma(\vec{r}, T, 0)$, the four linear equations with $B_i = 0$, $i > 2$, for a third estimate of $\Gamma(\vec{r}, T, 0)$, and so forth. We thus build up a table of estimates much like an ordinary Neville table.

We performed this extrapolation for $\Gamma(\vec{r}, T_C, 0)$ in an attempt to observe its large r behavior $\Gamma(\vec{r}, T_C, 0) \to D(0)/r^{1+\eta}$. The extrapolation at T_C is only rapidly convergent for seven of the nearest sites, $1 \le r/a \le 2.83$, which are not strictly asymptotic; however, if the asymptotic form is valid

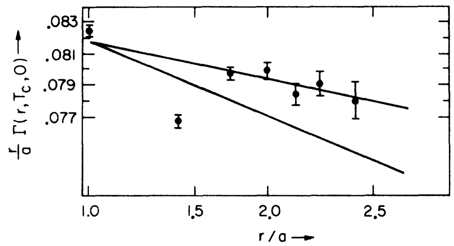

FIG. 1. Log-log plot of $r\Gamma(\vec{r}, T_C, 0)$ vs r. The value for $\vec{r}=a(\sqrt{2}, 0, 0)$, is well below the others and, thus, shows the same departures from spherical symmetry observed for this site in similar plots for the three-dimensional Ising model. The straight line of slope $-\eta=-0.04$ fits the data better than either the steeper line of slope -0.08 or r, the horizontal representing $\eta=0.00$.

here for as short a range as in the two-dimensional Ising model, these sites should determine η. Shown in Fig. 1 is a log-log plot of $r\Gamma(\vec{r}, T_C, 0)$ vs r for these sites. The uncertainties and departures from spherical symmetry limit our accuracy in determining η; however, the straight line of slope $-\eta=-0.040$ fits the data much better than either the steeper line representing $-\eta=-0.080$ or the horizontal representing $\eta=0.00$. Therefore, this determination is consistent with (if somewhat less accurate than) the assertion $\eta=0.040\pm 0.008$ of I.

Extrapolations for $\Gamma(\vec{r}, T, 0)$ were performed for $0.01\le\epsilon\le 0.08$ and for $1\le r/a\le\sqrt{10}$ including the 11 nearest sites, except $(a\sqrt{2}, 0, 0)$ which, as can be seen in Fig. 1, exhibits significant deviations from spherical symmetry. Figure 2 shows the results of these extrapolations in a semilog plot of $(r/a)^{1+\eta}\,\Gamma(\vec{r}, T, 0)/(\kappa r)^{\eta}$ vs $\kappa r=\kappa_0\epsilon^{\nu} r$. For large κr, $\Gamma(\vec{r}, T, 0)$ is believed to have the Ornstein-Zernike form $\kappa^{\eta}e^{-\kappa r}/r$. Thus, in the Ornstein-Zernike region, the values in Fig. 2 should be described by a straight line of slope -1.0. The values of the indices used were the ones determined in I, $\nu=0.717$ and $\eta=0.040$. The dependence does appear to be linear for the range of κr tested; there are few values for $\kappa r<0.02$. The value of $\kappa_0 a=2.50\pm 0.10$ was chosen so that the slope of the line would be -1.0; as we shall see, this value is consistent with the value determined directly from series.

III. TRUE CORRELATION LENGTH

Fisher and Burford have demonstrated that, at least for the zero-field spin-$\frac{1}{2}$ Ising system above T_C, there exists a unique solution of the equation $\Gamma^{-1}(\vec{k}, T, h=0)=0$ for k^2 as a power series in v.[3] Recently, Fisher and Camp have generalized this result.[7] This strengthens the long-held belief that the singularities of $\Gamma(\vec{k}, T, h)$ in the complex k plane, nearest $|k|=0$, are simple poles at $k=\pm i\kappa$. Fisher and Burford determined the solution using a diagrammatic prescription; however, it should be possible to find this solution using our correlation-function series. To this end, we derive $\Gamma^{-1}(\vec{k}, T, h)$ from our series.

Let us define

$$\Gamma(\vec{k}, T, h)=\sum_{\vec{r}} e^{i\vec{k}\cdot\vec{r}}\,\Gamma(\vec{r}, T, h)$$

$$=\sum_{i,j}\sum_{\vec{r}} e^{i\vec{k}\cdot\vec{r}} v^i h^j Q(\vec{r}, i, j)\;, \tag{3.1}$$

where we have derived all the $Q(\vec{r}, i, j=0)$ for $i\le 10$ and all the $Q(\vec{r}, i, j=2)$ for $i\le 8$. We are working with the fcc lattice whose lattice sites are uniquely determined by the prescription $\vec{r}=(a/\sqrt{2})\times(l, m, n)$ for all integers l, m, n such that $l+m+n$ is an even integer, a being the nearest-neighbor distance. Therefore, like several other cubic lattices, the fcc is symmetric upon reflection in the plane defined by any cube face. Because of this symmetry, Eq. (3.1) can be transformed so that the sum is only over one octant of the lattice,

$$\Gamma(\vec{k}, T, h)=\sum_{l=0}^{\infty}\sum_{m=0}^{\infty}\sum_{n=0}^{\infty}\sum_{i=0}^{\infty}\left(2\cos k_x\frac{la}{\sqrt{2}}\right)\left(2\cos k_y\frac{ma}{\sqrt{2}}\right)\left(2\cos k_z\frac{na}{\sqrt{2}}\right)\sum_{j=0}^{\infty} v^i h^j Q\left(\frac{a}{\sqrt{2}}(l, m, n), i, j\right)\;. \tag{3.2}$$

Using the relation between $2\cos lx$ and the $(2\cos x)^m$, for all $m\le l$, in Eq. (3.2), it is straightforward to find the coefficients $q(l, m, n, i, j)$ in the series

$$3\Gamma(\vec{k}, T, h)=\sum_{l,m,n,i,j}\left(2\cos\frac{k_x a}{\sqrt{2}}\right)^l\left(2\cos\frac{k_y a}{\sqrt{2}}\right)^m\left(2\cos\frac{k_z a}{\sqrt{2}}\right)^n v^i h^j q(l, m, n, i, j)\;. \tag{3.3}$$

Again, it is straightforward to find the inverse of (3.3),

$$\tfrac{1}{3}\Gamma^{-1}(\vec{k}, T, h)=\sum_{l,m,n,i,j}\left(2\cos\frac{k_x a}{\sqrt{2}}\right)^l\left(2\cos\frac{k_y a}{\sqrt{2}}\right)^m\left(2\cos\frac{k_z a}{\sqrt{2}}\right)^n v^i h^j \mathcal{H}(l, m, n, i, j)\;. \tag{3.4}$$

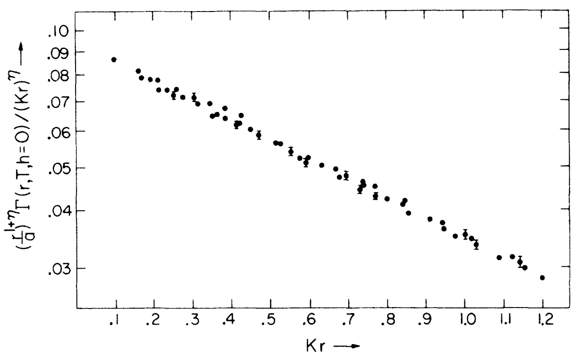

FIG. 2. Semilog plot of $(r/a)^{1+\eta}\Gamma(\vec{r}, T, 0)/(\kappa r)^{\eta}$ vs r for $0.01 \le \epsilon \le 0.08$ and for ten sites $\vec{r}$, where $1 < r/a < \sqrt{10}$. The values of the variables used in this plot are $\nu = 0.717$, $\eta = 0.040$, and $\kappa_0 a = 2.50$.

We have chosen to present our series in this form, Table I, partly because it is useful in finding the true correlation length but primarily for reasons of economy. For $i \le 10$, $Q((a/\sqrt{2})(l,m,n),i,j)$ is nonzero for 122 inequivalent sites $\vec{r}$, while to the same order $\mathcal{K}(l,m,n,i,j)$ is nonzero for only nine inequivalent sites. It should not be hard for the reader to reverse the above procedure so that he might find $\Gamma(\vec{r},T,h)$ and, consequently, all the series analyzed in I.

Before we proceed to find an iterative solution for the true correlation length, we must choose a direction for the solution and determine how the solution is affected by unknown terms in the series $\Gamma^{-1}(\vec{k},T,h=0)$. The equation can be solved for $i\kappa$ in any chosen direction. After Fisher and Burford, we choose to consider correlations in the (1, 0, 0) direction:

$$\tfrac{1}{3}\Gamma^{-1}(\vec{k}=(k,0,0),T,h=0)$$

$$=\sum_{l,i} v^i \left(2\cos\frac{ka}{\sqrt{2}}\right)^l H(l,i); H(l,i)$$

$$=\sum_{m,n} 2^{m+n}\mathcal{K}(l,m,n,i,j=0)\ . \qquad (3.5)$$

By requiring that the coefficient of zeroth order in v of $\Gamma^{-1}(i\kappa,T,h=0)$ be zero, we find, from Table II, $2\cos(i\kappa a/\sqrt{2}) = 3/4v$. This lowest order in the solution was derived assuming that the unknown terms $H(n,i,j=0)$ for $i>10$ could be neglected; but we see that, if nonzero, $H(11,11,0)$ will contribute to zeroth order in $\Gamma^{-1}(i\kappa,T,0)$. However, it can be shown by diagrammatic arguments that, if $n>1$, $H(n,i,j\neq 0)$ is zero for $i<2n$ and that $H(n,i,0)$ is zero for $i<3n$. The arguments leading to these results are rather complicated and will be more appropriately treated elsewhere.[8] Hence, the lowest unknown order in $\Gamma^{-1}(i\kappa,T,0)$, that is $[2\cos(i\kappa a/\sqrt{2})]^n H(n,i,0)$, is v^8 coming from both $H(3,11,0)$ and $H(4,12,0)$, allowing us to correctly determine eight terms in the iterative solution for $2\cos(i\kappa a/\sqrt{2})$. We find the next term in the solution by requiring that the coefficient of v in $\Gamma^{-1}(i\kappa,T,0)$ be zero:

$$\tfrac{1}{3}\Gamma^{-1}(i\kappa,T,0) = 1 - \tfrac{4}{3}v + \tfrac{4}{3}v^2 + \cdots$$
$$- (\tfrac{4}{3}v + \cdots)(3/4v + b + \cdots) + \cdots$$
$$= -\tfrac{4}{3}v(1+b) + \cdots\ . \qquad (3.6)$$

Thus $2\cos i\kappa a/\sqrt{2} = 3/4v - 1 + \cdots$. We can proceed in this manner to find the first eight terms of the solution. Shown in Table III is a rearrangement of this solution,

$$\Lambda = \frac{1}{2\cos(i\kappa a/\sqrt{2}) - 2} \to \frac{2}{(\kappa a)^2} \quad \text{as } \kappa \to 0\ .$$

Since κ is the inverse correlation length $\kappa = 1/\xi = \kappa_0\epsilon^{\nu}$, Λ should diverge as $2/(\kappa_0 a\epsilon^{\nu})^2$ (the same singularity as $\mu_2/3\chi$, also shown in Table III).

Shown with these series in Table III are Neville tables of the ratio sequence $n\rho_n v_C - n + 1$ [sequence (2.3) of I] and of the log-derivative sequence [Eq. (2.5) of I] for the series Λ and $\mu_2/3\chi$ using T_C

TABLE II. Shown are the coefficients $H(l,i,j=0)$ of the series, Eq. (3.5), for $\tfrac{1}{3}\Gamma^{-1}(\vec{k}=(k,0,0),T,h=0)$.

l	$H(l,i,0)$			
0	$+1.0$	$-1.333\,333\,333v$	$+1.333\,333\,333v^2$	$+1.718\,518\,519v^3$
	$+2.992\,592\,593v^4$	$+5.949\,065\,257v^5$	$+12.724\,499\,31v^6$	$+29.103\,123\,13v^7$
	$+70.231\,468\,49v^8$	$+175.989\,216\,4v^9$	$+453.093\,743\,9v^{10}$	
1	$-1.333\,333\,333v$	$+0.0v^2$	$-0.059\,259\,259\,3v^3$	$-0.237\,037\,037\,0v^4$
	$-0.687\,971\,781\,3v^5$	$-1.852\,651\,381v^6$	$-4.855\,513\,489v^7$	$-12.628\,411\,22v^8$
	$-33.010\,528\,50v^9$	$-86.953\,750\,99v^{10}$		
2	$-0.021\,947\,873\,8v^6$	$-0.140\,349\,337\,0v^7$	$-0.617\,477\,997\,7v^8$	$-2.372\,944\,844v^9$
	$-8.437\,318\,363v^{10}$			
3	$-0.012\,869\,583\,0v^9$	$-0.140\,945\,018\,7v^{10}$		

TABLE III. Presented are the series Λ and $\mu_2/3\chi$, analysis of these series for 2ν using Neville tables of sequences (2.3) and (2.5) of I with $T_C = 3.1753$, analysis for $\kappa_0 a$ using Neville tables of sequence (3.7) with $T_C = 3.1753$ and $\nu = 0.718$, and the series $\phi = \Lambda/(\mu_2/3\chi) - 1$, which is a measure of the departure from Ornstein Zernike.

n	Λ					$\mu_2/3\chi$				
1	1.333 333 333 333 3					1.333 333 333 333 3				
2	5.333 333 333 333 3					5.333 333 333 333 3				
3	19.614 814 814 815					19.614 814 814 815				
4	69.451 851 851 852					69.451 851 851 852				
5	240.467 396 749 62					240.450 934 744 27				
6	820.333 676 660 79					820.228 414 658 04				
7	2769.377 179 437 0					2768.907 563 394 0				
8	9276.891 068 188 9					9275.010 726 114 4				
9						30 882.974 301 814				
10						102 341.800 227 98				
	2ν from sequence (2.3) of I, $n\rho v_C - n + 1$									
4	1.4604									
5	1.4520	1.4184								
6	1.4461	1.4168	1.4135			1.4458				
7	1.4423	1.4189	1.4240	1.4380		1.4420	1.4191			
8	1.4396	1.4216	1.4296	1.4388		1.4394	1.4214	1.4287		
9						1.4376	1.4234	1.4303	1.4334	
10						1.4363	1.4251	1.4316	1.4345	
	2ν from sequence (2.5) of I									
4	1.3660									
5	1.3836	1.4541								
6	1.3931	1.4408	1.4142			1.3927				
7	1.3995	1.4374	1.4289	1.4486		1.3992	1.4380			
8	1.4042	1.4373	1.4374	1.4514		1.4040	1.4374	1.4357		
9						1.4077	1.4374	1.4372	1.4403	
10						1.4107	1.4376	1.4383	1.4409	
	$\kappa_0 a$ from sequence (3.7)									
1	2.6153					2.6153				
2	2.5716					2.5716				
3	2.5572					2.5572				
4	2.5502	2.5292				2.5502	2.5292			
5	2.5465	2.5315	2.5349			2.5465	2.5319	2.5360		
6	2.5444	2.5344	2.5403	2.5458		2.5446	2.5439	2.5411	2.5462	
7	2.5434	2.5370	2.5433	2.5473	2.5484	2.5436	2.5375	2.5438	2.5474	2.5483
8	2.5428	2.5389	2.5449	2.5476	2.5480	2.5431	2.5390	2.5456	2.5485	2.5495
9						2.5429	2.5411	2.5468	2.5492	2.5501
10						2.5428	2.5424	2.5476	2.5496	2.5503

$\phi = 0.012\,345\,678\,9v^4 + 0.029\,563\,786\,1v^5 + 0.052\,338\,232\,4v^6 + 0.122\,914\,782\,7v^7$

$= 3.1753$. The limits of these sequences for both series should be 2ν; and, indeed, taking proper account of the uncertainty in T_C, we would assert $2\nu = 1.436 \pm 0.014$ or $\nu = 0.718 \pm 0.007$ in good agreement with the result of I, $\nu = 0.717 \pm 0.007$. We determine $\kappa_0 a$ using the traditional method,[6] as follows. Since the series

$$\Lambda = \sum_{n=0}^{\infty} \lambda(n) v^n$$

has

$$\frac{2}{(\kappa_0 a)^2 \epsilon^{2\nu}} = \frac{2}{(\kappa_0 a)^2} \sum_{n=0}^{\infty} \frac{\Gamma(n+2\nu)}{\Gamma(n+1)\Gamma(2\nu)} \left(\frac{v}{v_C}\right)^n ,$$

where $\Gamma(n)$ is the familiar Γ function, as its leading singularity, the limit of the sequence

$$[2\Gamma(n+2\nu)/\Gamma(n+1)\Gamma(2\nu)\lambda(n)\, v_C^n]^{1/2} \tag{3.7}$$

is $\kappa_0 a$. The Neville tables of this sequence for the two series Λ and $\mu_2/3\chi$ are shown in Table III. From these it can be seen that $2.535 < \kappa_0 a < 2.550$; when proper account is taken of the uncertainties in T_C and ν, we assert $\kappa_0 a = 2.545 \pm 0.020$. This value is somewhat larger than, but not inconsistent with, the one determined from the extrapolation of $\Gamma(\vec{r}, T, 0)$ in Sec. II.

IV. FISHER-BURFORD PARAMETRIZATION

If the correlation function were exactly of the Ornstein-Zernike form $f(T)/(k^2 + \kappa^2)$, $f(T)$ being some function of T, then the series Λ would equal $\mu_2/3\chi$. As was observed by Fisher and Burford for the spin-$\frac{1}{2}$ Ising model, the series

$$\phi = \frac{\Lambda}{\mu_2/3\chi} - 1 ,$$

shown in Table III, which is a measure of departure from Ornstein Zernike, begins with fourth order in v, is termwise small, and appears to be convergent.

We now consider the approximant to $\Gamma(\vec{k}, T, h=0)$ which uses series we have already presented, as suggested by Fisher and Burford. This approximant[3] is

$$\Gamma(\vec{k}, T, h=0) = \chi\left(1 + \frac{2\phi}{\eta}\frac{\Lambda}{2}(\mathcal{K}a)^2\right)^{\eta/2} \Big/ \left(1 + \frac{\Lambda}{2}(\mathcal{K}a)^2\right). \quad (4.1)$$

$(\mathcal{K}a)^2 = 6[1 - (1/q)\sum_{\vec{\delta}} e^{i\vec{k}\cdot\vec{r}}]$, where the sum is over the q nearest-neighbor lattice sites $\vec{\delta}$; this variable has both the symmetry of the lattice, so that $\Gamma(\vec{k}+\vec{G}, T, 0) = \Gamma(\vec{k}, T, 0)$ for $\vec{G}$ (a reciprocal lattice vector) and the appropriate limiting behavior $(\mathcal{K}a)^2 \to (ka)^2$ as $k^2 \to 0$. For the fcc lattice and for $\vec{k} = (k, 0, 0)$, $(\mathcal{K}a)^2 = 4 - 4\cos(ka/\sqrt{2})$. ϕ is included in the approximant in such a way that the second moment of the approximant exactly equals the second moment of the correlations. This parametrization has the following advantages: It has the proper simple pole structure, and its zeroth and second moments equal χ and μ_2, respectively.

Near the critical point $k \to 0$, $T \to T_C$, this approximant takes the form

$$\Gamma(\vec{k}, T, 0) = \chi\left(1 + \frac{2}{\eta}\phi\Big|_{T_C}\frac{k^2}{\kappa^2}\right)^{\eta/2} \Big/ \left(1 + \frac{k^2}{\kappa^2}\right). \quad (4.2)$$

We have determined the properties of all the parameters of Eq. (4.2) except

$$\phi\Big|_{T=T_C} = \sum_{n=0}^{N} \phi_n v_C^n .$$

Using the ratio method [sequence (2.3) of I] with $T_C = 3.1753$ on this four-term series, we find the sequence -0.299, -1.66, -0.882, which, although badly behaved, is consistent with the assumption that ϕ is convergent. Forming the partial sums

$$\phi\Big|_{T=T_C}^{N} = \sum_{n=0}^{N} \phi_n v_C^n ,$$

one finds the sequence 0.000 12, 0.000 21, 0.000 26, 0.000 30; for this sequence, the linear extrapolants are 0.000 58, 0.000 52, 0.000 53, which indicate that $\phi|_{T=T_C}$ is quite small. Of course, the series is very badly behaved; but it is still hard to believe that ϕ is divergent or that $\phi|_{T=T_C} > 0.001$. Using this upper bound $(2/\eta)\phi|_{T=T_C} = 0.05$ in Eq. (4.2), we have

$$\frac{\kappa^{-2+\eta}(1 + 0.05\,k^2/\kappa^2)^{\eta/2}}{1 + k^2/\kappa^2} .$$

This should be well approximated by the Ornstein-Zernike form $\kappa^\eta/(k^2+\kappa^2)$ except for large k^2/κ^2; for $k^2/\kappa^2 < 12$ the discrepancy is less than 1%. These deviations for large k^2/κ^2 correspond to the deviations observed for small κr, $\kappa r < 0.1$.

V. CONCLUSION

From examination of our series we have found that, except for distances much smaller than a coherence length, the Ornstein-Zernike form approximates well the critical spin-spin correlations. As discussed in I, the results of a neutron scattering experiment on $RbMnF_3$ agree well with our predictions for γ and ν; but, for η, the experiment indicates that $\eta = 0.067 \pm 0.010$, whereas we believe that $\eta = 0.040 \pm 0.008$.[9] However, Corliss *et al.* assumed that $\Gamma(\vec{k}, T, 0) = (k^2+\kappa^2)^{\eta/2}/(k^2+\kappa^2)$ in fitting their data. This approximation assumes that the Fisher-Burford parameter $\phi|_{T=T_C} = 1$ rather than $\phi|_{T=T_C} = 0$ of Ornstein Zernike which is much closer to the model results. We argue that their form will opt for an excessively high value of η because, for fixed k^2 and η, $(k^2+\kappa^2)^{\eta/2}$ will vary more slowly with κ than will κ^η. Hence, to indicate the same variation, $(k^2+\kappa^2)^{\eta/2}$ requires a higher value of η than does κ^η.

---

†Research supported in part by the National Science Foundation under Grant No. NSF GP-16886.

*Xerox Corporation Industrial Fellow.

[1]M. Ferer, M. A. Moore, and Michael Wortis, preceding paper, Phys. Rev. B 4, 3954 (1971).

[2]L. P. Kadanoff, Nuovo Cimento 44b, 276 (1966).

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

[4]M. A. Moore, D. Jasnow, and M. Wortis, Phys. Rev. Letters 22, 940 (1969); M. Ferer, M. A. Moore, and M. Wortis, *ibid.* 22, 1382 (1969).

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

[6]M. E. Fisher, Rept. Progr. Phys. 30, 615 (1967).

[7]W. J. Camp and M. E. Fisher, Phys. Rev. Letters 26, 73 (1971).

[8]M. Ferer, M. A. Moore, and M. Wortis (unpublished). This paper will be a lengthy consideration of correlations, primarily for the spin-$\frac{1}{2}$ Ising model. Among other things that will be considered are the diagrammatic arguments mentioned in Sec. III of the present paper, and investigation of the angular dependence of $i\kappa$, and a quantitative comparison of the parametrization of Sec. IV with extrapolations similar to those of Sec. II.

[9]L. M. Corliss, A. Delapalme, J. M. Hastings, H. Y. Lau, and R. Nathans, J. Appl. Phys. 40, 1278 (1969).